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# THERMODYNAMIC EQUILIBRIUM

## IN PREBIOLOGICAL

## ATMOSPHERES OF

## C, H, O, N, P, S, AND Cl

DAYHOFF, LIPPINCOTT,  
ECK, and NAGARAJAN

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By M. O. Dayhoff, E. R. Lippincott,  
R. V. Eck, and G. Nagarajan

National Biomedical Research Foundation  
and  
The University of Maryland

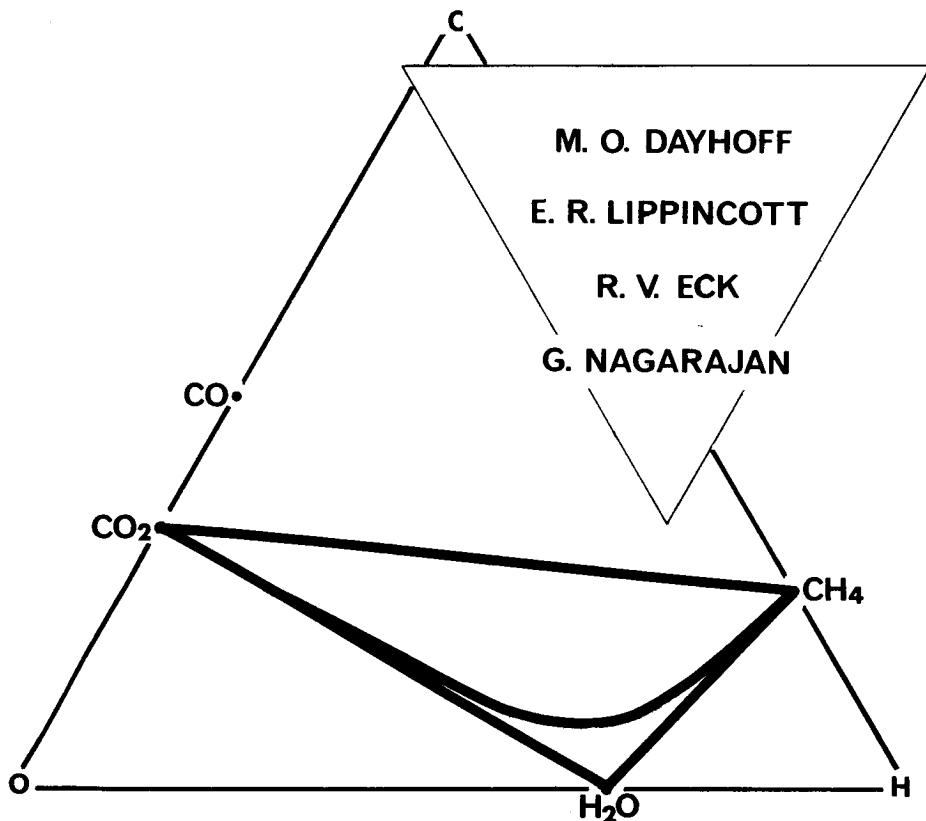
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7 1967

# THERMODYNAMIC EQUILIBRIUM in PREBIOLOGICAL ATMOSPHERES of C, H, O, N, P, S, and Cl



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## FOREWORD

The original suggestion that a chemical equilibrium approach could contribute to an understanding of the origin of life on the earth and other planets was made by Harold Morowitz of Yale University, who felt that the quantitative results so derived could be valuable in lending substance to this highly speculative and controversial field. Toward this end, this book presents a survey of thermodynamic equilibrium states of ideal gas systems containing C, H, O, N, P, S, and Cl. This book also presents the mathematical methods used and describes the computer program by means of which the tables were derived.

There are many applications and uses for the survey presented here. In exobiology, the results can be utilized for investigating the inorganic origin of organic matter and establishing criteria for the presence of life on other planets; in biology, restricted thermodynamic equilibrium studies can contribute to a knowledge of the balance of individual equilibrium systems that occur within the cell; in astronomy, the results can be applied to investigations of the atmospheres of celestial bodies and their evolution; in synthetic chemistry, thermodynamic equilibrium states can be predicted under various conditions; in petroleum chemistry, investigations of the optimum conditions for obtaining desired petroleum derivatives can be carried out theoretically; in geology, inferences can be drawn concerning the past conditions of the earth and the origin of the solar system from investigations of which equilibrium states can produce substances actually found in the earth or in meteorites; and in combustion engineering, studies can be made of jet fuels and the components of the exhausts of jet engines. (The basic methods used in this project had previously been developed by others for application to fuel combustion.)

The book is divided into five sections. The first chapter presents an introduction to the methods and gives the tables which comprise the computer survey. The second chapter describes the mathematical methods utilized. The third chapter gives the computer program which produced the results. This program, originally written by M. O. Dayhoff, was translated to Fortran IV by Chan Mo Park. Two appendixes give applications of the survey to research problems: Appendix I, by E. R. Lippincott, R. V. Eck, M. O. Dayhoff, and Carl Sagan, discusses applications with regard to the thermodynamic equilibria in planetary atmospheres; and Appendix II, by R. V. Eck, E. R. Lippincott, M. O. Dayhoff, and Y. T. Pratt, discusses applications with regard to the role of thermodynamic equilibrium in the inorganic origin of organic matter.

In parallel with this project, the thermodynamics group at the National Bureau of Standards, under the direction of George Armstrong, who also reviewed this report, has been collecting the thermodynamic data for organic compounds, particularly those ubiquitous to life on earth. Much of the essential data has not been measured for these compounds, and those values that are available are scattered throughout the literature.

This work was supported by Contract No. NSR 21-003-002 to the National Biomedical Research Foundation and Grant No. NGR 21-002-059 to the University of Maryland, both from the National Aeronautics and Space Administration. The research of Appendix I was also supported in part by NASA Grant No. NGR 09-015-023 with the Smithsonian Astrophysical Observatory. The computations were made at the University of Maryland Computer Science Center.

Robert S. Ledley, President  
National Biomedical Research Foundation

## CONTENTS

	Page
FOREWORD . . . . .	iii
LIST OF FIGURES . . . . .	vii
LIST OF TABLES . . . . .	viii
GLOSSARY OF SYMBOLS . . . . .	xi
<b>1. THERMODYNAMIC EQUILIBRIUM IN ATMOSPHERES OF C, H, O, N, P, S, AND Cl</b>	
Introduction . . . . .	1
The C, H, O System . . . . .	4
Systems of C, H, O, N, P, S, Cl . . . . .	7
Discussion of Data Presented . . . . .	12
Ternary Diagrams . . . . .	12
Concentrations of Compounds at Seven Elemental Compositions . . . . .	14
Partial Molal Free Energies of the Elements . . . . .	14
Standard Free Energies of Formation . . . . .	14
References . . . . .	15
Data Presentation . . . . .	16
Ternary Diagrams, Tables of Partial Molal Free Energy of Elements, and Tables of Compound Concentrations for Various Systems . . . . .	17
Table of the Standard Free Energies of Formation of Organic and Inorganic Compounds . . . . .	154
Table of the Standard Free Energies of Formation of Atomic Groups . . . . .	166
Examples of the Calculation of the Standard Free Energies of Formation of Compounds . . . . .	170
<b>2. DESCRIPTION OF COMPUTATIONAL METHODS</b>	
Gibbs Free Energy Function . . . . .	171
Standard Free Energy of Formation . . . . .	171
Definition of Standard States . . . . .	172
Estimation of Free Energies from Group Contributions . . . . .	172
Equilibrium Constants from Free Energies . . . . .	173
Calculation of Chemical Equilibrium in Complex Mixtures . . . . .	175
Calculation of Compound Concentrations from Tables of Partial Molal Free Energies . . . . .	178
Concentration Dependence of the Partial Molal Free Energies . . . . .	179
Errors Due to Uncertainties in Free Energy Values . . . . .	183
Metastable Systems . . . . .	184
References . . . . .	187

## 3. PROGRAM CHEM-EQUILIBRIUM

Program Description . . . . .	189
Subprogram Listing . . . . .	191
Subprogram Linkage . . . . .	192
Data Card Formats . . . . .	193
Listing of Fortran IV Statements . . . . .	197
Listing of Sample Data Deck . . . . .	218

## APPENDIX I

## THERMODYNAMIC EQUILIBRIA IN PLANETARY ATMOSPHERES

*E. R. Lippincott, R. V. Eck, M. O. Dayhoff, and Carl Sagan*

Abstract . . . . .	219
Introduction . . . . .	220
Methods of Calculation . . . . .	221
Observational Limitations . . . . .	222
The Earth . . . . .	222
Venus . . . . .	225
Evolution of the Atmosphere of Venus . . . . .	231
Mars . . . . .	233
Jupiter . . . . .	235
References . . . . .	240

## APPENDIX II

## THERMODYNAMIC EQUILIBRIUM AND THE INORGANIC ORIGIN OF ORGANIC COMPOUNDS

*R. V. Eck, E. R. Lippincott, M. O. Dayhoff, and Y. T. Pratt*

Abstract . . . . .	243
Introduction . . . . .	243
C, H, O Systems . . . . .	245
Method of Limited Equilibrium, Exclusion of Graphite . . . . .	248
C, H, O, N, S, P, Cl, Systems . . . . .	250
Application to Observed Data . . . . .	253
Plasma Experiments . . . . .	255
References . . . . .	257

SUBJECT INDEX . . . . .	259
-------------------------	-----

## LIST OF FIGURES

	Page
1. Thermodynamic equilibria in atmospheres of varying elemental proportions . . . . .	5
2. Graphite phase boundaries . . . . .	8
3. Curves where benzene concentration is $10^{-6}$ mole fraction . . . . .	10
4. Curves above which asphalt concentration is $10^{-6}$ mole fraction . . . . .	11
Ternary diagrams showing concentrations of compounds in systems of varying C, H, O composition	

Page	Page		
5. Hydrogen, diatomic . . . . .	19	35. Cyanic acid . . . . .	51
6. Oxygen, diatomic . . . . .	20	36. Methylamine . . . . .	52
7. Water . . . . .	21	37. Dimethylamine . . . . .	53
8. Carbon monoxide . . . . .	22	38. Aniline . . . . .	54
9. Carbon dioxide . . . . .	23	39. Pyrrole . . . . .	55
10. Methane . . . . .	24	40. Pyridine . . . . .	56
11. Benzene . . . . .	25	41. Pyrimidine . . . . .	57
12. Naphthalene . . . . .	26	42. Purine . . . . .	58
13. Asphalt . . . . .	27	43. Urea . . . . .	59
14. Xylene . . . . .	28	44. Formamide . . . . .	60
15. Furan . . . . .	29	45. Ethanolamine . . . . .	61
16. Ethane . . . . .	30	46. Glycine . . . . .	62
17. Hexane . . . . .	31	47. Phenylalanine . . . . .	63
18. Cyclohexane . . . . .	32	48. Phosphorus trioxide, dimeric . . . . .	66
19. Ethylene . . . . .	33	49. Phosphorus pentoxide, dimeric . . . . .	67
20. Acetylene . . . . .	34	50. Phosphine . . . . .	68
21. Methanol . . . . .	35	51. Chlorine, diatomic . . . . .	69
22. Ethanol . . . . .	36	52. Hydrogen chloride . . . . .	70
23. Acetaldehyde . . . . .	37	53. Chloromethane . . . . .	71
24. Formic acid . . . . .	38	54. Hydrogen sulfide . . . . .	72
25. Acetic acid . . . . .	39	55. Sulfur dioxide . . . . .	73
26. Oxalic acid . . . . .	40	56. Sulfur trioxide . . . . .	74
27. Nitrogen, diatomic . . . . .	43	57. Carbonyl sulfide . . . . .	75
28. Ammonia . . . . .	44	58. Carbon disulfide . . . . .	76
29. Hydrazine . . . . .	45	59. Methanethiol . . . . .	77
30. Nitrogen dioxide . . . . .	46	60. Benzenethiol . . . . .	78
31. Nitric acid . . . . .	47	61. Thiophene . . . . .	79
32. Hydrogen cyanide . . . . .	48	62. Dimethylsulfide . . . . .	80
33. Cyanogen . . . . .	49	63. Cysteine . . . . .	81
34. Cyanamide . . . . .	50		

## APPENDIX I

1. C-H-O ternary diagram for the Cytherean atmosphere . . . . .	226
2. C-H-O ternary diagram enlarged one hundredfold . . . . .	228
3. Evolution of the atmosphere of Venus . . . . .	232
4. C-H-O ternary diagram for the Martian atmosphere . . . . .	234

## APPENDIX II

1. Thermodynamic equilibria in atmospheres of varying elemental proportions . . . . .	246
2. Graphite phase boundaries . . . . .	247
3. Curves where benzene concentration is $10^{-6}$ mole fraction . . . . .	249
4. Curves above which asphalt concentration is greater than $10^{-6}$ mole fraction . . . . .	251
5. Compounds detected in products of plasma discharge reactions . . . . .	256

LIST OF TABLES

	Page
Partial molal free energies of the elements (a) and equilibrium concentrations of selected compounds (b) are presented for the following systems:	
1. 500°K, 0.2 atm. pressure, C, H, O system . . . . .	17
2. 500°K, 1 atm. pressure, C, H, O, N system where N constitutes 80% of the total number of moles of all elements . . . . .	41
3. 500°K, 0.2 atm. pressure, C, H, O, N, P, S, Cl system where N, P, S, and Cl each constitute .01% of the total number of moles of all elements . . . . .	64
Partial molal free energies of the elements (a) and equilibrium concentrations of selected compounds (b) for systems of C, H, O, and N. N constitutes 80% of the total number of moles in the system. Results are presented under each of the following conditions:	
4. 300°K and $1 \times 10^{-3}$ atm. pressure . . . . .	82
5. 300°K and 1 atm. pressure . . . . .	84
6. 300°K and 100 atm. pressure . . . . .	86
7. 500°K and $1 \times 10^{-3}$ atm. pressure . . . . .	88
8. 500°K and 1 atm. pressure . . . . .	90
9. 500°K and 100 atm. pressure . . . . .	92
10. 700°K and $1 \times 10^{-3}$ atm. pressure . . . . .	94
11. 700°K and 1 atm. pressure . . . . .	96
12. 700°K and 100 atm. pressure . . . . .	98
13. 1000°K and $1 \times 10^{-3}$ atm. pressure . . . . .	100
14. 1000°K and 1 atm. pressure . . . . .	102
15. 1000°K and 100 atm. pressure . . . . .	104
Partial molal free energies of the elements (a) and equilibrium concentrations of selected compounds (b) for systems of C, H, O, N, P, S, and Cl. N, P, S, and Cl each constitute .01% of the total number of moles in the system. Results are presented under each of the following conditions:	
16. 300°K and $0.2 \times 10^{-3}$ atm. pressure . . . . .	106
17. 300°K and 0.2 atm. pressure . . . . .	108
18. 300°K and 20 atm. pressure . . . . .	110
19. 500°K and $0.2 \times 10^{-3}$ atm. pressure . . . . .	112
20. 500°K and 0.2 atm. pressure . . . . .	114
21. 500°K and 20 atm. pressure . . . . .	116
22. 700°K and $0.2 \times 10^{-3}$ atm. pressure . . . . .	118
23. 700°K and 0.2 atm. pressure . . . . .	120
24. 700°K and 20 atm. pressure . . . . .	122
25. 1000°K and $0.2 \times 10^{-3}$ atm. pressure . . . . .	124
26. 1000°K and 0.2 atm. pressure . . . . .	126
27. 1000°K and 20 atm. pressure . . . . .	128

Partial molal free energies of the elements (a) and equilibrium concentrations of selected compounds (b) for systems of C, H, O, N, P, S, and Cl. N, P, S, and Cl each constitute 0.0001% of the total number of moles in the system. Results are presented under each of the following conditions:

	Page
28. 300°K and $0.2 \times 10^{-3}$ atm. pressure . . . . .	130
29. 300°K and 0.2 atm. pressure . . . . .	132
30. 300°K and 20 atm. pressure . . . . .	134
31. 500°K and $0.2 \times 10^{-3}$ atm. pressure . . . . .	136
32. 500°K and 0.2 atm. pressure . . . . .	138
33. 500°K and 20 atm. pressure . . . . .	140
34. 700°K and $0.2 \times 10^{-3}$ atm. pressure . . . . .	142
35. 700°K and 0.2 atm. pressure . . . . .	144
36. 700°K and 20 atm. pressure . . . . .	146
37. 1000°K and $0.2 \times 10^{-3}$ atm. pressure . . . . .	148
38. 1000°K and 0.2 atm. pressure . . . . .	150
39. 1000°K and 20 atm. pressure . . . . .	152
40. Standard free energies of formation for various organic and inorganic compounds at four temperatures . . . . .	154
41. Standard free energies of formation for various groups of atoms at four temperatures . . . . .	166
42. Calculations of standard free energies of formation by the group contribution method for anthracene, glycine, and cyclohexane . . . . .	170
43. Partial molal free energies and partial pressures for three characteristic systems at 500°K and 1 atm. pressure . . . . .	180
44. Dependence of partial molal free energies of trace constituents upon elemental concentrations . . . . .	182
45. Concentration change with change in free energy of formation . . . . .	183
46. Mole fractions of major constituents in systems with and without graphite at 500°K and 1 atm. pressure . . . . .	185
47. Effect of the number of aromatic compounds in the equilibrium on the partial molal free energies and compound concentrations . . . . .	186

#### APPENDIX I

1. Adopted chemical composition and physical parameters of the terrestrial atmosphere . . . . .	223
2. Thermodynamic equilibrium composition of the terrestrial atmosphere . . . . .	223
3. Adopted chemical composition of the Cytherean atmosphere . . . . .	230
4. Thermodynamic equilibrium composition of the Cytherean atmosphere . . . . .	230
5. Adopted chemical composition of the Martian atmosphere . . . . .	236
6. Thermodynamic equilibrium composition of the Martian atmosphere . . . . .	236
7. Adopted chemical composition of the Jovian atmosphere . . . . .	237
8. Thermodynamic equilibrium composition of the Jovian atmosphere . . . . .	237
9. Predicted equilibrium in the Jovian atmosphere at high temperatures and moderate to low pressures . . . . .	239

APPENDIX II

1. Mole fraction compositions of compounds in equilibrium . . . . . 252
2. Mole fraction composition of gas mixtures with graphite or graphite and aromatics omitted from the equilibrium . . . . . 254

## GLOSSARY OF SYMBOLS

R	gas constant, 1.9864 cal./mole degree
F	Gibbs free energy function
$\Delta F$	free energy change during a reaction
$\Delta F^{\circ}$	standard free energy change during a reaction
E	internal energy function
S	entropy
H	enthalpy
$\Delta F_i^{\circ}$	standard free energy of formation of compound i
$f_i$	total free energy of one chemical species in the ideal gas mixture
$K_p$	equilibrium constant based on partial pressures
$F(X)$	total free energy of a system of i compounds, each present in concentration $X_i$
$\bar{F}_j$	partial molal free energy of element j in the system
P	pressure of total system in atmospheres
V	volume
T	temperature in degrees Kelvin
$P_i$	partial pressure of the $i^{\text{th}}$ compound
$X_i$	total number of moles of the $i^{\text{th}}$ compound
$\bar{X}$	total number of moles in the system
$B_j$	total number of moles of element j in the system
$A_{ij}$	number of atoms of element j in compound i

## SUBSCRIPTS

i	compound i
j	element j
n	total number of compounds in the system
m	total number of elements in the system

**Chapter 1**  
**Thermodynamic Equilibrium**  
**in Atmospheres of**  
**C, H, O, N, P, S, and Cl**

## CHAPTER 1

### THERMODYNAMIC EQUILIBRIUM IN ATMOSPHERES OF C, H, O, N, P, S, AND Cl

#### Introduction

One of the major problems in understanding prebiological conditions on the earth and in the atmospheres of extraterrestrial bodies is the nature of the complex chemical species which might be encountered. Some kinds of organic compounds must have been available for the origin, structure, and nutrition of the first living things. These compounds must have been produced by nonliving processes in suitable quantities and proportions. The understanding of their formation is one essential component in a detailed, rational theory of the evolution of chemical reactions and of the origin of life.

It has long been recognized that equilibrium processes are important in determining what compounds are present in atmospheres, particularly where high temperatures, suitable catalysts, or long time periods are involved. Under conditions where special mechanisms, such as radiation or lightning, operate to favor production of certain compounds, there will also be a tendency to form products required by thermodynamic equilibrium. Compounds which can be formed at equilibrium need no special mechanism to explain their presence. However, such special mechanisms would have to be sought for those compounds which could not be so produced but which would have been required for the structure of the first living things.

The computed concentrations and proportions of compounds which would be produced by simple equilibrium processes would be an interesting and useful basis for the comparison of any experiments, observations, or theories concerning special mechanisms. For example, it would be interesting to compare the proportions of various amino acids produced by electric discharge in simulated atmospheres with the corresponding proportions computed for equilibrium, even though the absolute amounts might be different.

A computational system for the equilibrium of many compounds in an ideal gas mixture was developed as a first stage. The results may be used in more complex models; for example, a dynamic equilibrium might be simulated by two systems at equilibrium under different conditions, with a restricted exchange between them. Other stages would include condensed and polyphase systems.

Equilibrium computations may be used to simulate rate-limited kinetic systems. The formation of certain products whose activation energies are high is precluded by omitting the compounds from the computation. All the remaining compounds are considered to be at complete equilibrium. If done carefully, making plausible assumptions, such computations can be made to approximate possible physical situations.

This book has to do with the first stage of this project, in which the systems computed are simple ideal gas mixtures.

There have been previous computations of equilibrium concentrations of major constituents in particular reactions. A number of these were summarized by Miller and Urey (1959) and by Oparin (1957). More recently, equilibria in the system C H O in regions up to the graphite phase boundary have been considered by Suess (1962), for several different temperatures and pressures, but for a limited number of compounds. Cairns and Tevebaugh (1964) have made similar computations for 1 atm. pressure and temperatures of 298 to 1500°K. Heald, Naughton and Barnes have made calculations of universal equilibria in volcanic gases for a C H O S system (1963).

Until the present time, there has been no unified study of chemical equilibria in gaseous systems containing a large number of organic compounds of the elements C, H, O, N, P, S, and Cl. In their calculations of the general C H O system, previous authors have not considered the metastable region above the graphite phase boundary. However, Dayhoff, Lippincott and Eck (1964) presented the calculated distribution of elements among over 100 C H O compounds, at 1 atm. and 500°K. The characteristics of these systems throughout a broad range of temperatures, pressures, and elemental compositions are of great interest in the fields of biology and exobiology, astronomy, synthetic chemistry, petroleum chemistry, geology, and combustion engineering. The main results of a more extensive survey are presented here. In addition, methods and tables are presented which permit subsequent calculations of the concentrations of additional trace compounds not tabulated here. A detailed description of how this can be done is presented in Chapter 2. Appendix I describes the application of thermodynamic methods to the study of the composition and evolution of planetary atmospheres. Appendix II describes a thermodynamic approach to the inorganic origin of organic compounds in such materials as carbonaceous chondrites.

The difficulties previously restricting the scope of the computation of concentrations of organic compounds at equilibrium have recently been overcome by the use of the high-speed electronic computer. Our own program, written for the IBM 7094 computer is based on a very general method developed by White, Johnson, and Dantzig (1958), that of minimizing the free energy of the entire system in order to determine the equilibrium balance of species. The solution is approached by an iterative process. At each step, ( $M+1$ ) linear equations are solved, where  $M$  is the number of elements in the system. Thousands of concentrations can be calculated and organized for convenient display in only one minute of computer time. The method used is described in Chapter 2, where, in addition, equations used in the text are derived. The computer program is described and listed in Chapter 3.

The concept of chemical thermodynamic equilibrium makes possible a useful approximation in many practical situations. The distribution of molecular species which it yields is independent of the rates or nature of the specific reactions by which equilibrium was reached. It is only necessary to assume that

there is at least one reversible reaction path from the major constituents to each other compound. The final concentrations of species depend only on the pressure, temperature, and elemental composition of the whole system and are a function of the molecular formulae and the standard free energies of formation of the compounds present. The equilibrium constants for all possible individual reactions are then simultaneously satisfied in the complex mixture.

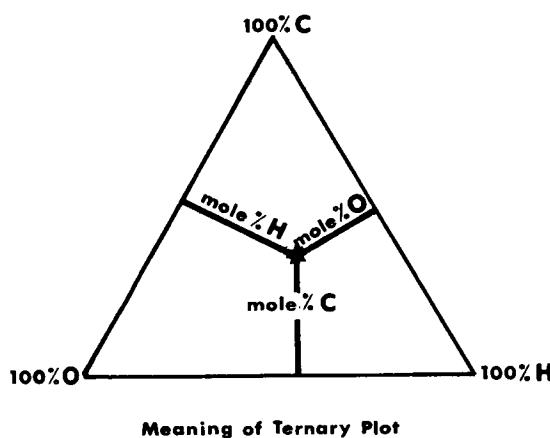
The lower homologues of all the more stable chemical families are explicitly included in our computations. With the exception of aromatic compounds in a limited region, concentrations of the high homologues of all families fall off rapidly with increasing size. However, the number of isomers of each compound increases with an increase in the chain length. For a saturated hydrocarbon of 20 carbon atoms, there are almost one million isomers. These isomers can be considered as a single "composite" compound, whose concentration is equal to the sum of concentrations of all the component isomers. Such composites can then be included in the computations. For hydrocarbons of 20 carbon atoms, even the total concentration of the million isomers is still quite negligible.

The perspective one obtains in considering a large number of diverse kinds of compounds at one time is quite different from that derived from ordinary mass balance equations, although the answers must agree. Our computational method is formulated in a general way, and therefore is entirely independent of the particular compounds in any given equilibrium. These compounds are specified for each particular chemical system by means of a single data card for each constituent. With such a computational method, it becomes easy to omit one or more major constituents and to determine the balance of species in the remaining, limited system. Some results of this technique are discussed in the paper which constitutes Appendix II, in which restrictions were made on aromatic and asphaltic compounds. Under some conditions, for example fairly low temperatures, some reactions may be so slow that their products fail to form in quantity during the time available. Such a condition is simulated by deleting the slow-forming products from the inputs. The balance of chemical species may then be remarkably different from that in the unrestricted system. For example, if graphite cannot be produced, polynuclear aromatics form. If these are also inhibited, aliphatic hydrocarbons, cyclohexane, butadiene, and related compounds become important. As another example, HCN, pyridine, and other nitrogen heterocyclics are produced in the presence of nitrogen. If N<sub>2</sub> itself is forbidden, the concentrations of these nitrogenous compounds are enhanced.

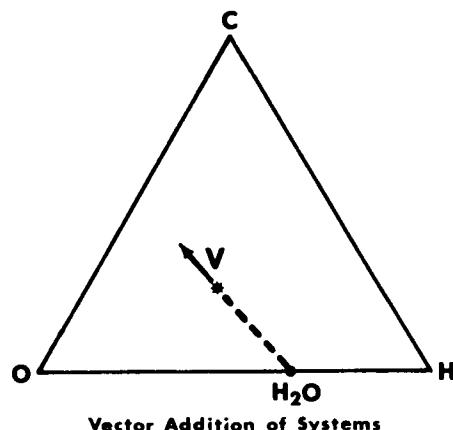
The limited equilibrium method thus assumes that the rates of all reactions leading to an excluded compound are zero while all the included compounds form rapidly. Such a gross approach to kinetics can only be approximate. However, a useful qualitative picture of those compounds which may be important under some special circumstances can be obtained. The minimal set of restrictions necessary to account for each of these compounds can also be determined.

## The C H O System

The ternary diagram provides a particularly useful means of displaying the characteristics of ideal gaseous systems containing all proportions of elements C, H, and O. For every point in such a diagram, the mole fraction of each element is proportional to the perpendicular distance to the corresponding side.



Meaning of Ternary Plot



Vector Addition of Systems

With the ternary diagram it is quite easy to see the effect of removal from or addition to a system of one compound (or any mixture of fixed composition). The composition of all systems along any line in the diagram can be represented as the sum of the compositions of varying proportions of any two distinct systems on the line. Thus, if H<sub>2</sub>O is removed from the system plotted at \*, the composition of the resultant system lies at the end of a vector V as shown in the right-hand diagram. The length of the vector depends on the quantity removed.

The main characteristics of ideal gas systems containing all proportions of C, H, and O are shown in Fig. 1. There are two pronounced thresholds at which the concentrations of many compounds change abruptly by many orders of magnitude. The first of these is the oxygen threshold along the CO<sub>2</sub>-H<sub>2</sub>O line. Below this line in the oxygen region, free oxygen appears and all organic compounds are fully oxidized. Above it, traces of many organics appear in addition to CO<sub>2</sub>, CO, H<sub>2</sub>O, and CH<sub>4</sub>. The second is the asphalt threshold above which large concentrations of benzene and polynuclear aromatics appear. The position of this threshold varies with pressure and temperature, in contrast to the oxygen threshold which remains essentially unchanged. At 500°K and 1 atm. pressure, the asphalt threshold lies along the CH<sub>4</sub>-CO<sub>2</sub> line, as shown. There is also a weak hydrogen threshold along the CH<sub>4</sub>-H<sub>2</sub>O line which appears at low temperatures.

According to a formally strict definition of thermodynamic equilibrium, graphite must be included as a major constituent of the system. In Fig. 1., the solid curve shows the graphite phase boundary at 500°K and 1 atm. pressure. Below this curve the concentrations of all organic compounds except CH<sub>4</sub> and CO<sub>2</sub> are very small. Graphite is the end product of the polymerization of higher aromatic compounds, a relatively slow sequence of reactions. At temperatures below 1000°K,

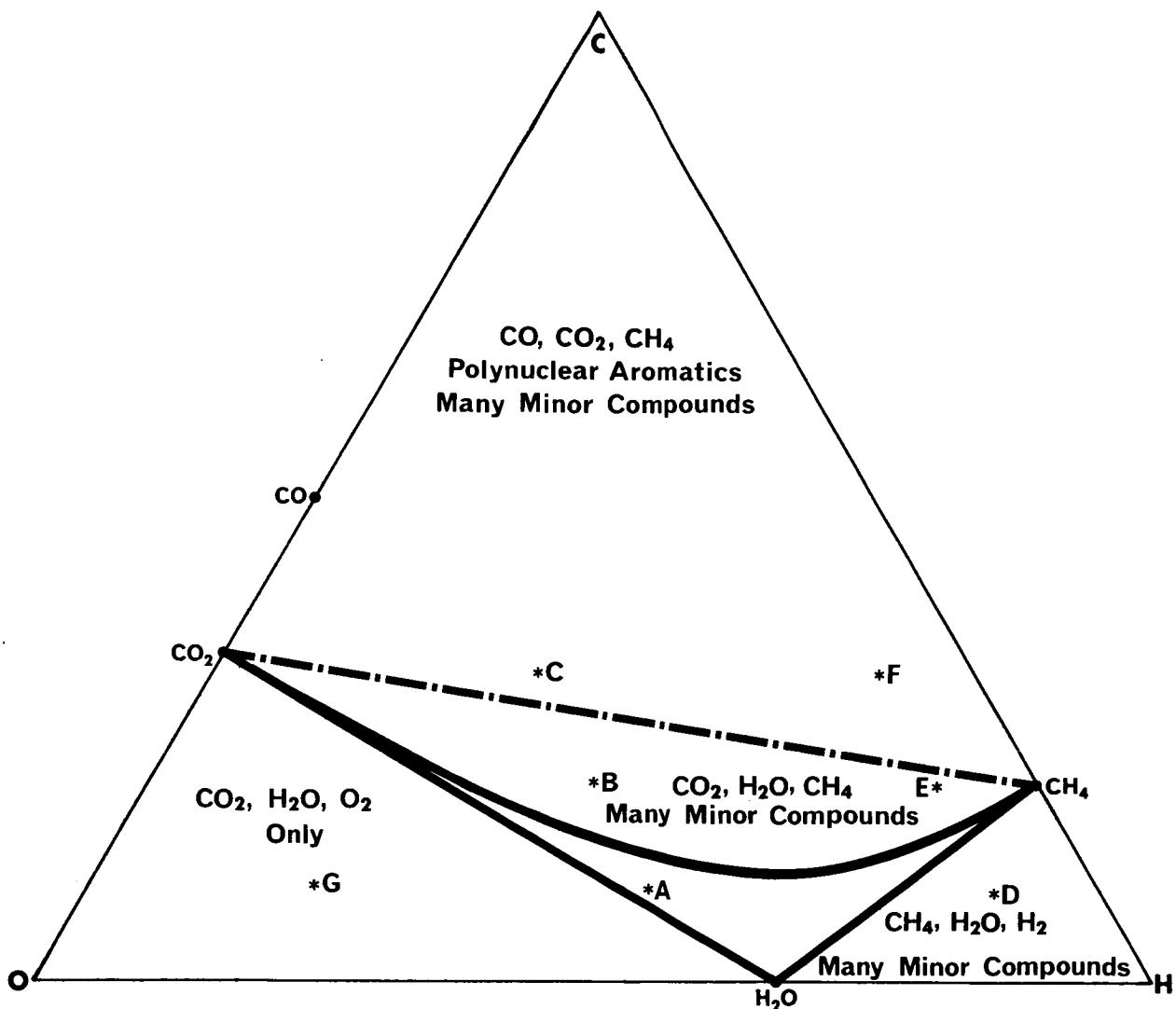
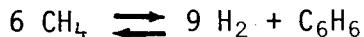


Fig. 1. Thermodynamic equilibria in atmospheres of varying elemental proportions. The ternary diagram provides a display of systems of all possible relative proportions of C, H, and O. The points corresponding to atmospheres of pure gases of the major compounds are indicated and regions where different compounds are important are shown. The solid curve indicates the phase boundary along which graphite becomes stable at 1 atm. pressure and 500°K. The activation energy for this reaction is so high that under many conditions it does not occur and gaseous equilibria above this line are observed. Above the line  $\text{CH}_4\text{-CO}_2$ , equilibrium favors the formation of large proportions of polycyclic aromatic compounds or asphalts and a lesser increase in most of the other families of compounds. The graphite and asphalt lines are always present, but their position varies with temperature and pressure. The points A through G indicate the system compositions used in Tables 1 through 39 part-b. A represents a system with C:H:O ratio 10:50:40; B, 20:40:40; C, 30:30:40; D, 10:80:10; E, 20:70:10; F, 30:60:10; and G, 10:20:70.

it usually does not form immediately from methane and other simple organics, because the activation energies of the intermediate reactants would be too high. At moderate temperatures, it is reasonable and instructive to presume that a metastable equilibrium of other compounds would be approached before significant amounts of graphite were produced. The elemental proportions represented by the region above the graphite line in the ternary diagram therefore give experimentally attainable gas-phase compositions. The exclusion of graphite permits these compositions to be studied, and the "asphalt region" to be investigated.

The positions of the graphite phase boundary at various temperatures and pressures are shown in Fig. 2. Any system whose composition lies in the upper part of these ternary diagrams would form two phases, graphite and a gas. The composition of the gas phase is determined by the intersection of the graphite line and a line projected from the carbon corner through the system composition point.

In order to investigate the characteristics in the metastable system above the graphite phase line, graphite is excluded from the computations. In Fig. 3, concentration boundaries are shown for benzene. Above these lines the benzene concentration is greater than  $10^{-6}$  mole fraction, an amount readily measured experimentally. At high temperatures and low pressures, benzene (and asphalt) appear even in an atmosphere containing a large excess of free hydrogen -- a result consistent with the experimental findings of Studier, Hayatsu, and Anders (1965) in heat-catalysed reactions and with those of Lippincott and Pratt (Eck, Dayhoff, Lippincott, and Pratt, 1966) in quenched plasmas. Two mutually reinforcing factors lead to this effect: first, methane becomes less stable with increasing temperatures, and second, equations leading to aromatics, such as



shift toward the right as the pressure decreases. Benzene becomes measurable only in regions where solid graphite would be stable if it had been included in the equilibrium.

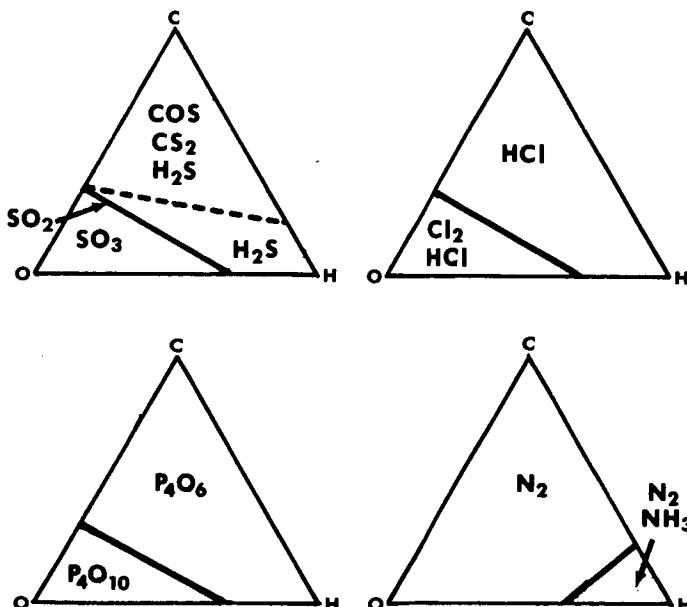
With graphite formation excluded, the concentrations of the other constituents change gradually in the neighborhood of the graphite line; it is not a definite threshold. Above the graphite line there are regions where the computed total mass of aromatic compounds becomes very high. The largest polynuclear aromatics become the most important, often so concentrated that they would precipitate. It is impossible then to include specifically every compound of this family. However, since the large molecules must build up from the small ones, the kinetic properties in a given situation dictate how far this polymerization will be able to go in the available time. We have approximated the condensation of polynuclear aromatics by including in our system benzene, naphthalene, and a mixture we call "asphalt", which is a composite of 100 isomers having six benzene rings with the molecular formula  $\text{C}_{22}\text{H}_{12}$ . The free energy of this composite is extrapolated from that of benzene and naphthalene by the method of group contributions, as formulated by van Krevelen and Chermin (1951). The position of the asphalt threshold, where aromatics build up sharply, is insensitive to the exact formulas and free energies of the aromatics included in the equilibria. The

dependence of the system on the nature of the aromatics included is discussed in Chapter 2, page 184. The threshold is sharper at low temperatures and at high pressures. Fig. 4 shows lines above which the asphalt concentration is greater than  $10^{-6}$  mole fraction, for various conditions of temperature and pressure. Asphalt may form at all temperatures and pressures investigated. At high temperature and low pressure, it is stable even where excess hydrogen is present.

A lowering of temperature of the system at point R in Fig. 4a would result in the precipitation of complex polynuclear aromatics. Similarly, (see Fig. 4b) as the pressure is lowered in a gaseous system at point Q, initially at 1 atm. pressure, polynuclear aromatics would be produced. In astronomical or geological contexts, a very simple change in environment might lead to the inorganic production of large molecules. Such aromatics are observed in carbonaceous meteorites.

#### Systems of C, H, O, N, P, S, Cl

For nitrogen and the elements S, P, and Cl in low concentrations, only a few compounds are important. Those which account for 0.1% or more of each element are shown below in the regions in which they appear.



Nitrogen is quite inert, occurring in most systems almost exclusively as N<sub>2</sub>. Even when it is a major fraction of the mixture, only small amounts of other nitrogenous compounds usually occur. However, at extreme conditions of low temperatures and high pressures, in the region where there is free hydrogen, NH<sub>3</sub> becomes the main nitrogen-containing compound. Small amounts of HCN and pyridine form in the asphalt region. Traces of nitrogen-containing organics appear everywhere except in the oxygen region, where there are traces of the oxides of nitrogen.

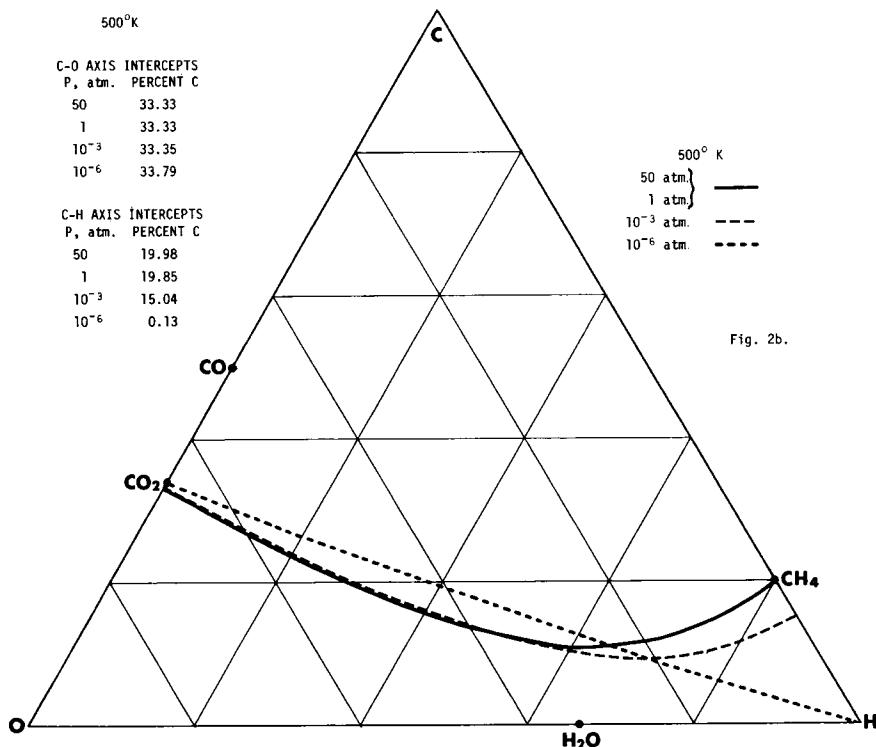
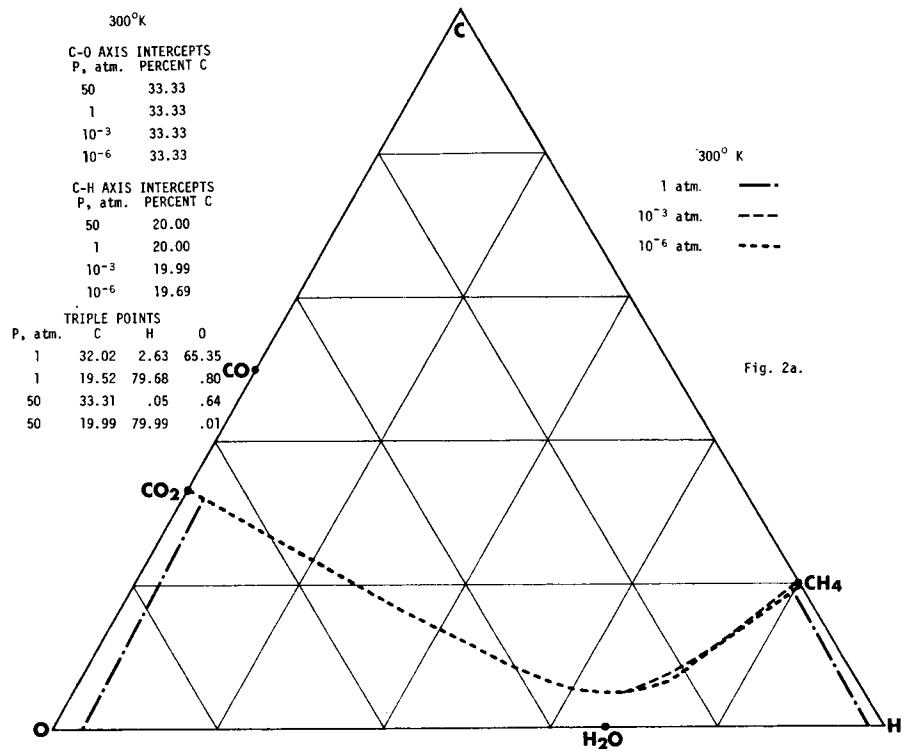
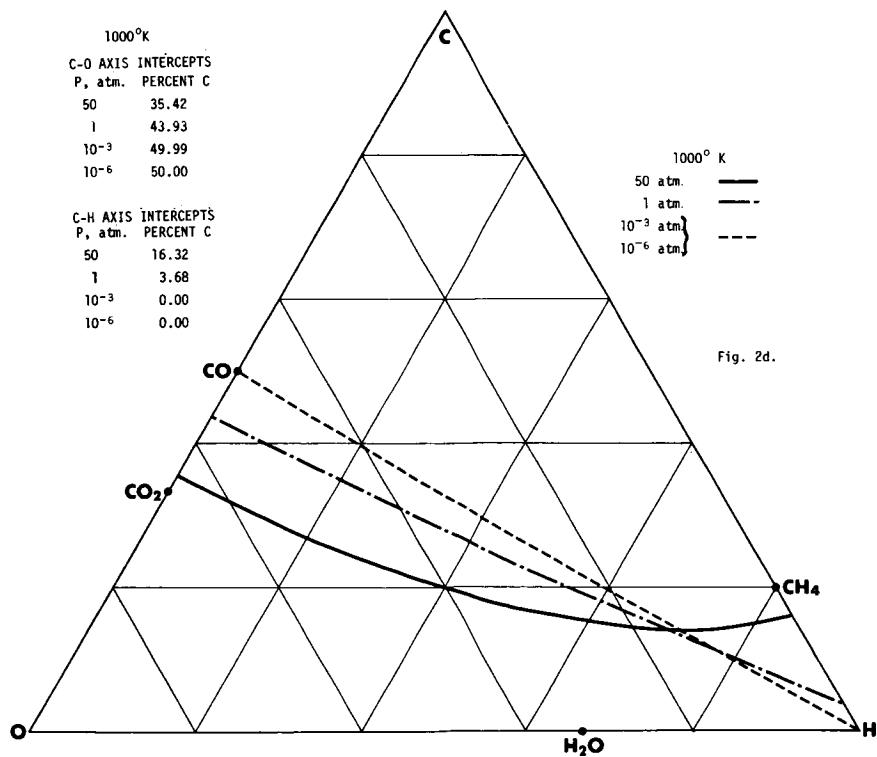
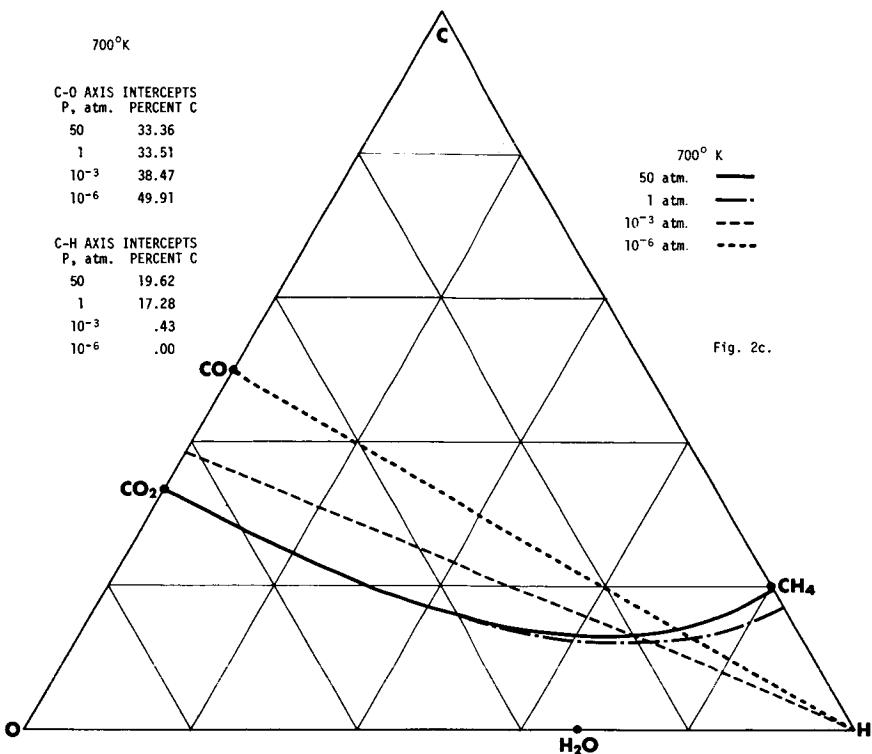


Fig. 2. Graphite phase boundaries. In an all-inclusive equilibrium, the gas phase would never have a composition above this phase boundary. A system whose total composition fell in the upper part of the triangle would precipitate graphite. The gas phase composition would be given by the point of intersection of the graphite phase line and a line projected from the carbon corner through the system composition point. The activation energy barrier to graphite formation is very high so that under many conditions equilibrium may actually be approximated in metastable gases without any graphite formation.



In diagram 2a at 300°K, a liquid water phase forms in addition to graphite at 1 and 50 atm. pressure. Two triple points are possible. At low temperatures and moderate pressures the graphite lines pass through the  $\text{CO}_2$  and  $\text{CH}_4$  points. At higher temperatures and lower pressures this boundary extends to the hydrogen corner as shown in Figs. 2b, 2c and 2d. Numerical values of the phase boundary are shown for the two component systems C/O and C/H.

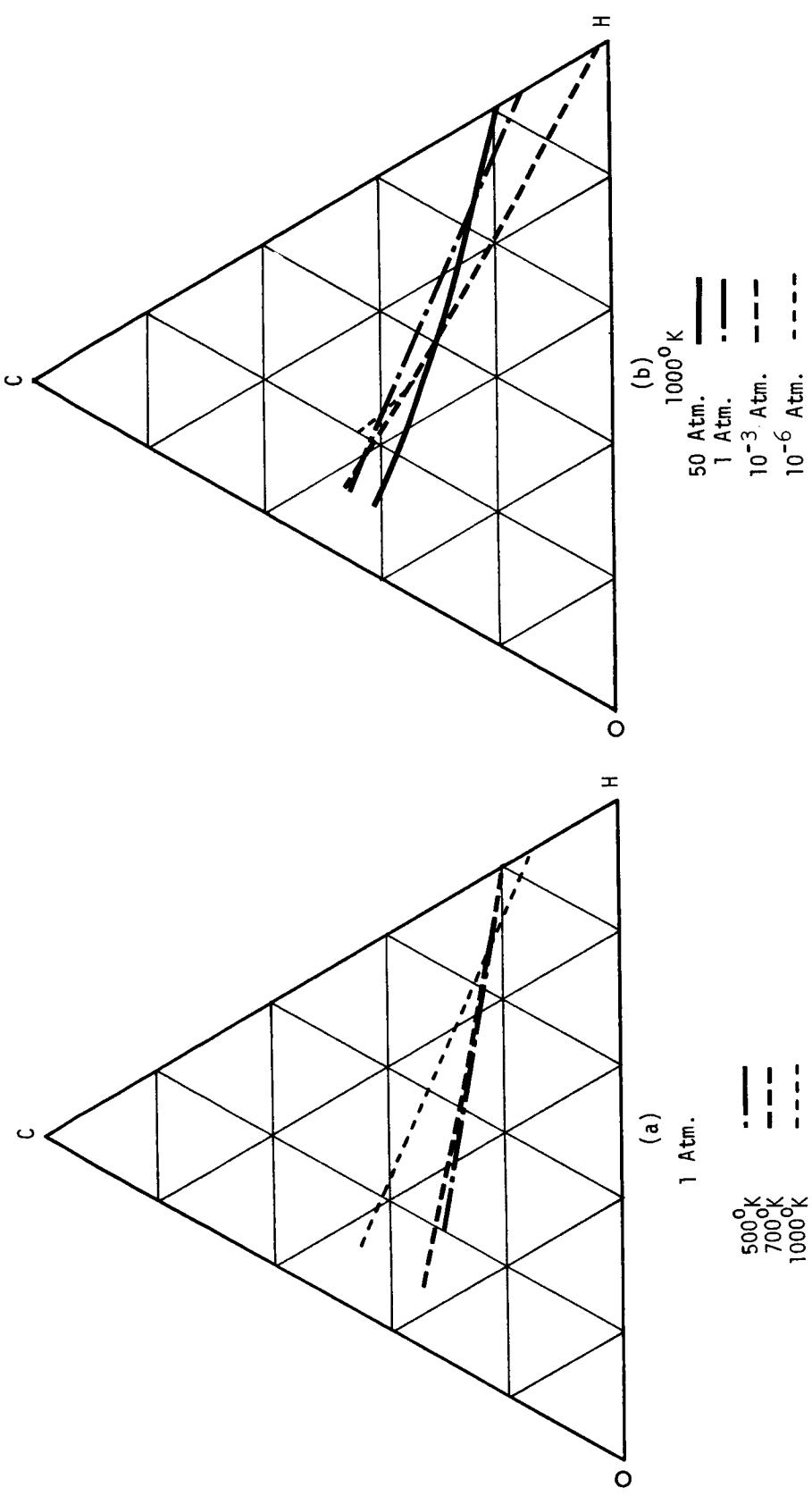


Fig. 3. Curves where benzene concentration is  $10^{-6}$  mole fraction. Benzene is found at  $1000^{\circ}\text{K}$  even in the presence of an excess of hydrogen. In the diagram (a) at  $300^{\circ}\text{K}$  the benzene concentration is slightly lower than  $10^{-6}$  atm. pressure above the  $\text{CO}_2\text{-CH}_4$  line and much lower elsewhere. The  $500^{\circ}\text{K}$  line is almost independent of pressure in the region  $10^{-3}$  to  $50$  atm. pressure. In diagram (b), the curves for  $10^{-3}$  atm. pressure and  $10^{-6}$  atm. pressure at  $1000^{\circ}\text{K}$  are indistinguishable except for the slight divergence at the upper end.

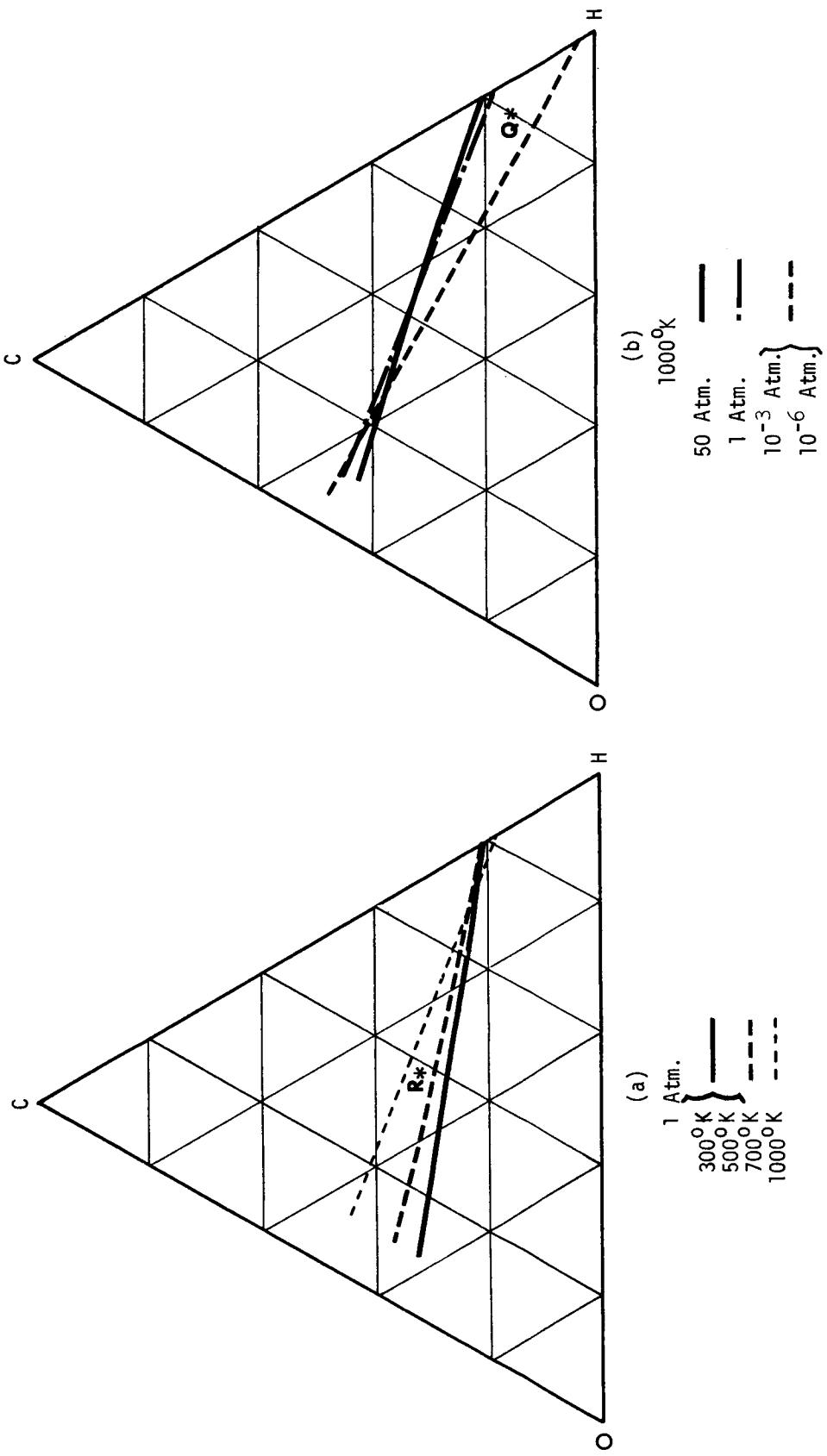


Fig. 4. Curves above which asphalt concentration is greater than  $10^{-6}$  mole fraction. Graphite has been omitted from these systems for kinetic reasons. Asphalt forms at all temperatures and pressures investigated. At high temperature and low pressure it is stable even where excess  $\text{H}_2$  is present. At  $300^{\circ}\text{K}$  the curves for pressures from  $10^{-6}$  to  $50$  atm. pressure are very close together. A system at  $R$  would contain only small molecular weight compounds at  $1000^{\circ}\text{K}$ . Lowering the temperature to  $700^{\circ}\text{K}$  would result in asphalt formation. Similarly, a system at  $Q$  would contain only small molecular weight compounds at  $1$  atm. pressure. A reduction in pressure would result in asphalt precipitation.

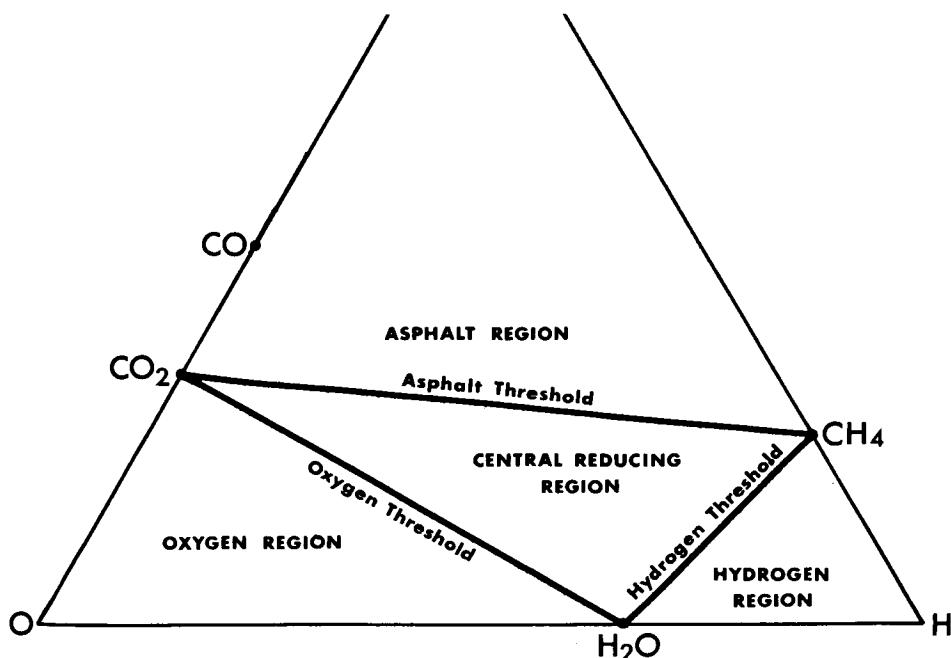
At low concentrations of chlorine this element exists as HCl in all the regions. Traces of oxides and acids of chlorine and free Cl<sub>2</sub> are also found in the oxygen region. The most stable organic, CH<sub>3</sub>Cl is found in trace amounts everywhere except the oxygen region. Chlorobenzene appears in the asphalt region.

Sulfur is found in many stable compounds. In the oxygen region, SO<sub>3</sub> is the principal compound. In the immediate vicinity of the oxygen threshold, SO<sub>2</sub> is very stable. Above the oxygen threshold, H<sub>2</sub>S is a main constituent. In the asphalt region, COS is important. Near the carbon corner, CS<sub>2</sub> reaches a high concentration. In general, the organic sulfur compounds are more stable than their oxygen analogues; for example, methanethiol is much more stable than methanol in systems of comparable sulfur and oxygen content.

#### Discussion of Data Presented

Ternary diagrams. In order to demonstrate the variation of the concentration of compounds in systems containing C, H, and O, we have presented a large number of ternary diagrams each showing the concentration of one compound in systems of varying elemental composition at 0.2 atm. and 500°K. These are shown in Figs. 5 to 26. Composition points for which computations were made are designated by an \*. This is followed by the mole fraction composition of the compound in that system. Values of <10<sup>-38</sup> are printed by the computer as "\*".

The interpretation of these diagrams is dependent on the main regions of the ternary diagram shown below. At the oxygen threshold, most compounds are reduced in concentration over many orders of magnitude. Organic compounds are essentially fully oxidized. At the asphalt threshold, in systems where graphite



has been excluded, there is a rapid increase in concentrations of polynuclear aromatics and their derivatives. There is also a less-pronounced change in the

concentrations of these compounds at the hydrogen threshold. There is no abrupt change within the central reducing region, even in the neighborhood of the graphite phase boundary.

From the ternary diagrams it can be seen that a compound has maximum concentration in a system close to its own elemental composition. Its concentration falls off very slowly in all triangles containing its composition point. There are usually abrupt changes in a constituent's concentration at the thresholds, beyond which its concentrations fall off slowly with distance from the composition point. The composition point of each compound is plotted on its diagram with a star, \*.

The conspicuous instability of all the common organic chemicals explains both the difficulty of obtaining stoichiometric yields in organic reactions at elevated temperatures and the accumulation of tars and carbon in reaction vessels. In practical laboratory experience, at room temperatures, the activation energies leading to the decomposition of these compounds are high, thus accounting for their thermodynamically metastable existence in our world.

The computations show that many common constituent compounds in biological systems are quite unstable, even in the asphalt region. Thus carbohydrates, sugars, fatty acids, glycerol, and proteins have nearly zero concentration in all the systems studied. Only in more limited equilibria, from which several stable compounds are excluded, is their presence appreciable. Actual realization of such limited equilibria is dependent on the availability of particular catalysts which would prohibit the formation of these more stable products while enhancing all other reaction rates.

In the systems studied here, the aromatic nitrogen compounds are less stable than the corresponding hydrocarbons. However, pyridine is relatively stable. If, in addition to graphite, aromatic hydrocarbons and  $N_2$  are excluded from the computations, pyridine, adenine, and other nitrogenous hydrocarbons become important. In actual practice such conditions can be realized over limited temperature ranges with particular catalysts.

Ternary diagrams for nitrogen compounds are taken from a system containing 80 mole percent nitrogen at 1 atm. pressure. Even under these encouraging elemental proportions, organic nitrogenous compounds are present only in very low concentrations. In the central reducing region, the order of decreasing stability of the amino acids is glycine, alanine, aspartic acid, serine, and valine. The others occur in less than  $10^{-37}$  mole percent concentration. (Figs. 27 to 47.)

The ternary diagrams for P, S, and Cl compounds are taken from systems with 0.01 mole percent of these elements added. This small amount does not perturb the C H O system measurably. For equivalent concentrations of S and O, the sulfur compounds are much more stable than their oxygen analogues. (Figs. 48 to 63.)

It may be noted that in the central reducing region,  $H_2S$ ,  $NH_3$ ,  $CH_4$ , and traces of the simple organic compounds observed in living cells are found. However, phosphorus is in the form  $P_4O_6$  (dehydrated phosphorus acid). This incompletely oxidized form of phosphorus is not commonly found in metabolism. On the other hand, at all points of stability for  $P_4O_{10}$  (anhydrous phosphoric acid),

$\text{H}_2\text{S}$ ,  $\text{NH}_3$ , and the organic compounds are completely oxidized. Some mechanisms must have been available in a primordial system to make such an unstable mixture available to life. Complete equilibrium seems to be incompatible with the simultaneous occurrence of the quantities and proportions of the various compounds necessary for the origin of life.

Concentrations of compounds at seven representative elemental compositions. The variation in the concentration of a particular compound is usually small within each region of the ternary diagram. We have therefore chosen to display the concentrations of many compounds at seven representative points, labeled A to G in Fig. 1, rather than to present their ternary diagrams in complete detail. The concentrations of these compounds at 500°K are listed in Tables 1b, 2b, and 3b. These tables are arranged so that homologous series appear together for comparison. Concentrations for C, H, and O compounds were determined in a system at 0.2 atm. pressure.

Since nitrogen is a very important constituent of organic compounds and since it is found in high concentration in the earth's atmosphere, we have tabulated the concentrations of the nitrogen-containing compounds in a system containing 80 mole percent nitrogen at 1 atm. pressure. Compounds containing N, P, S, and Cl were computed in systems at 0.2 atm. pressure containing 0.01 and 0.0001 mole percent of these elements. At these low concentrations these elements have negligible effect on each other or on the C H O system.

Concentrations of a smaller list of compounds are tabulated for 12 combinations of pressure and temperature. C H O systems with 80 mole percent nitrogen and with 0.01 and 0.0001 mole percent N, P, S, and Cl are shown in Tables 4b to 39b.

Partial molal free energies,  $\bar{f}$ . So far, we have characterized each system by its elemental composition. An additional powerful characterization is given by the partial molal free energies of the elements. These values are produced by the computational procedure described in Chapter 2. They are then used to calculate the concentrations of all the compounds in a system, according to Eq. (14) of Chapter 2. Since trace constituents do not perceptibly affect the  $\bar{f}$  values of a system, the concentration of any trace compound can later be calculated by hand from Eq. (14) of Chapter 2. For such a calculation, only the standard free energy of formation and the formula of the compound are needed.

We have therefore tabulated these characteristic  $\bar{f}$  values (in RT units) for each system studied, to permit later hand computation of the concentration of any compound. For an example, see Chapter 2. (See also Tables 1a to 39a.)

Standard free energies of formation. One major difficulty in dealing with organic compounds is the lack of reliable thermodynamic data. For the major as well as minor constituents on which measurements are available, we have used the JANAF Tables, the Petroleum Institute Research Project 44 Tables and the U. S. Bureau of Mines Bulletin No. 595.

Even an order of magnitude value is of significant interest for the minor constituents. Therefore, for many species we have used the approximation method of group contributions, as formulated by van Krevelen and Chermin (1951). In

this method, the standard free energy of a compound is considered to be composed of a sum of contributions from the bonds, steric configurations (as rings or branching), and the symmetry properties of the molecule. The values for the groups are derived from a set of compounds whose free energies have been measured.

In Table 40 we have presented the standard free energies of formation of 341 organic and inorganic compounds, at the four temperatures at which the computations for our tables have been made. Reference is made in the table to each source of information. From these values of free energy the concentration of any of these compounds over the range we consider can readily be calculated from Eq. (14) of Chapter 2.

In Table 41 we have presented the values which we have used for various groups in approximating their standard free energies of formation. Chapter 2 describes the use of these values. In Table 42 we have given an example of the actual calculations of the standard free energies of formation of anthracene, glycine, and cyclohexane at four temperatures.

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## DATA PRESENTATION

In Tables 1b to 39b, the distributions of compounds at equilibrium are shown for the following systems:

COMPOSITION POINT	MOLE FRACTION IN SYSTEM		
	C	H	O
A	10	50	40
B	20	40	40
C	30	30	40
D	10	80	10
E	20	70	10
F	30	60	10
G	10	20	70

The ternary diagrams show the concentration of one compound in systems of many elemental proportions. (See pages 4 and 12 for a discussion of ternary diagrams.) Composition points for which computations were made are designated by an \*. This is followed by the mole fraction composition of the compound in that system. Values less than  $10^{-38}$  are printed by the computer as "\*".

TABLE 1a

500°K AND 0.2 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  
 $\frac{F_j}{RT}$ , FOR 68 SYSTEMS OF C, H, AND O.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)		
	C	H	O	C	H	O
1	2.0	2.0	96.0	-98.160	-28.686	-0.837
2	2.0	9.0	89.0	-98.038	-27.894	-0.880
3	2.0	19.0	79.0	-97.831	-27.456	-0.955
4	2.0	29.0	69.0	-97.571	-27.165	-1.056
5	2.0	39.0	59.0	-97.219	-26.913	-1.202
6	2.0	49.0	49.0	-96.670	-26.645	-1.443
7	2.0	59.0	39.0	-95.354	-26.206	-2.066
8	2.0	69.0	29.0	-3.221	-2.275	-49.898
9	2.0	79.0	19.0	-7.573	-1.215	-52.577
10	2.0	89.0	9.0	-8.741	-0.954	-53.971
11	2.0	96.0	2.0	-9.237	-0.850	-55.763
12	10.0	2.0	88.0	-96.245	-28.588	-0.947
13	10.0	10.0	80.0	-96.048	-27.723	-1.022
14	10.0	20.0	70.0	-95.725	-27.281	-1.151
15	10.0	30.0	60.0	-95.259	-26.945	-1.354
16	10.0	40.0	50.0	-94.343	-26.555	-1.778
17	10.0	50.0	40.0	-6.689	-3.039	-48.632
18	10.0	60.0	30.0	-0.119	-2.803	-49.150
19	10.0	70.0	20.0	-0.328	-2.589	-49.638
20	10.0	80.0	10.0	-5.185	-1.354	-52.718
21	10.0	88.0	2.0	-6.637	-1.022	-55.116
22	20.0	2.0	78.0	-94.558	-28.410	-1.184
23	20.0	10.0	70.0	-94.566	-27.494	-1.354
24	20.0	20.0	60.0	-93.650	-26.901	-1.778
25	20.0	30.0	50.0	0.292	-3.276	-48.744
26	20.0	40.0	40.0	1.120	-3.109	-49.229
27	20.0	50.0	30.0	1.553	-3.054	-49.546
28	20.0	60.0	20.0	1.945	-3.038	-49.896
29	20.0	70.0	10.0	2.447	-3.071	-50.437
30	22.0	76.0	2.0	9.663	-4.806	-54.661
31	18.0	80.0	2.0	-1.690	-2.003	-52.719
32	30.0	2.0	68.0	-92.887	-27.960	-1.949
33	30.0	10.0	60.0	2.136	-3.730	-49.453
34	30.0	20.0	50.0	7.028	-4.582	-51.930
35	30.0	30.0	40.0	9.859	-5.177	-53.413
36	30.0	40.0	30.0	9.845	-5.082	-53.497
37	30.0	50.0	20.0	9.822	-4.995	-53.629
38	30.0	60.0	10.0	9.796	-4.912	-53.895
39	30.0	68.0	2.0	9.774	-4.845	-54.632
40	40.0	10.0	50.0	10.344	-5.926	-53.527
41	40.0	20.0	40.0	10.096	-5.446	-53.458
42	40.0	30.0	30.0	9.999	-5.245	-53.490
43	40.0	40.0	20.0	9.933	-5.101	-53.588
44	40.0	50.0	10.0	9.880	-4.978	-53.824
45	40.0	58.0	2.0	9.840	-4.885	-54.535
46	12.0	78.0	10.0	-3.722	-1.648	-52.025
47	14.0	76.0	10.0	-0.398	-2.420	-50.432
48	16.0	74.0	10.0	0.786	-2.692	-50.134
49	18.0	72.0	10.0	1.527	-2.860	-50.181
50	22.0	68.0	10.0	7.724	-4.372	-52.929
51	24.0	66.0	10.0	9.705	-4.872	-53.906
52	26.0	64.0	10.0	9.748	-4.888	-53.909
53	28.0	62.0	10.0	9.775	-4.900	-53.904
54	4.0	56.0	40.0	-94.342	-26.150	-2.222
55	6.0	54.0	40.0	-92.549	-25.818	-2.908
56	8.0	52.0	40.0	-1.380	-3.123	-48.371
57	12.0	48.0	40.0	-0.254	-3.019	-48.775
58	14.0	46.0	40.0	0.105	-3.022	-48.889
59	16.0	44.0	40.0	0.437	-3.038	-48.995
60	18.0	42.0	40.0	0.768	-3.067	-49.105
61	22.0	38.0	40.0	1.521	-3.169	-49.382
62	24.0	36.0	40.0	2.029	-3.260	-49.591
63	26.0	34.0	40.0	2.821	-3.425	-49.943
64	28.0	32.0	40.0	7.230	-4.498	-52.108
65	32.0	28.0	40.0	9.915	-5.218	-53.428
66	34.0	26.0	40.0	9.958	-5.260	-53.435
67	36.0	24.0	40.0	10.000	-5.309	-53.441
68	38.0	22.0	40.0	10.044	-5.368	-53.447

TABLE 1b

500°K AND 0.2 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, AND O WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O (SEE FIG. 1 FOR DETAILS).

COMPOUND	A	B	C	D	E	F	G
METHANE	3.5E-02	1.6E-01	2.6E-01	3.3E-01	7.2E-01	7.1E-01	0.
H2	1.1E-02	1.0E-02	1.6E-04	3.3E-01	1.1E-02	2.7E-04	1.0E-23
O2	0.	0.	0.	0.	0.	0.	5.0E-01
WATER	6.8E-01	3.3E-01	7.9E-05	3.3E-01	1.1E-01	8.3E-05	2.5E-01
CO	3.4E-05	1.2E-04	1.1E-02	6.4E-09	1.3E-04	6.4E-03	7.6E-26
CO2	2.7E-01	5.0E-01	7.2E-01	8.5E-07	1.7E-01	2.6E-01	2.5E-01
BENZENE	6.7E-27	2.3E-22	5.5E-05	3.2E-34	8.2E-19	1.9E-04	0.
NAPHTHALEN	0.	5.1E-36	3.0E-05	0.	4.1E-30	1.3E-04	0.
ASPHALT	0.	0.	4.5E-03	0.	0.	2.7E-02	0.
OZONE	0.	0.	0.	0.	0.	0.	4.8E-20
H2O2	6.2E-33	1.6E-33	6.1E-39	5.1E-35	1.6E-34	0.	9.5E-13
*OH	1.0E-25	5.3E-26	1.0E-28	9.4E-27	1.6E-26	8.2E-29	1.3E-15
C302	1.1E-37	7.2E-36	4.1E-28	0.	3.5E-35	1.3E-28	0.
ETHANE	4.7E-09	1.1E-07	1.8E-05	1.4E-08	2.0E-06	7.9E-05	0.
PROPANE	4.4E-15	5.7E-13	9.1E-09	4.4E-15	4.2E-11	6.3E-08	0.
BUTANE	8.8E-21	6.1E-18	9.6E-12	2.8E-21	1.8E-15	1.1E-10	0.
ISOBUTANE	1.0E-20	7.1E-18	1.1E-11	3.3E-21	2.1E-15	1.2E-10	0.
PENTANE	9.1E-27	3.3E-23	5.2E-15	9.5E-28	4.0E-20	9.3E-14	0.
HEXANE	1.1E-32	2.2E-28	3.4E-18	3.8E-34	1.1E-24	9.7E-17	0.
HEPTANE	1.3E-38	1.4E-33	2.1E-21	0.	2.7E-29	9.6E-20	0.
OCTANE	0.	8.2E-39	1.3E-24	0.	6.6E-34	9.2E-23	0.
CYCLOCRCANE	1.7E-22	2.6E-20	2.6E-14	5.9E-24	1.7E-18	1.0E-13	0.
CYCLOBUTANE	4.1E-24	3.2E-21	3.2E-13	4.5E-26	8.8E-19	2.1E-12	0.
CYCLOPENTANE	1.6E-27	6.9E-24	6.8E-14	5.9E-30	7.7E-21	7.1E-13	0.
CYCLOHEXANE	1.5E-32	3.3E-28	3.2E-16	1.7E-35	1.5E-24	5.4E-15	0.
ETHYLENE	2.5E-14	7.1E-13	7.1E-09	2.7E-15	1.2E-11	1.8E-08	0.
PROPENE	1.2E-18	1.7E-16	1.7E-10	4.0E-20	1.2E-14	7.0E-10	0.
BUTENE	1.6E-24	1.3E-21	1.3E-13	1.8E-26	3.5E-19	8.3E-13	0.
CCTENE	0.	0.	8.0E-27	0.	6.1E-38	3.4E-25	0.
ACETYLENE	5.6E-24	2.1E-22	1.3E-16	2.4E-26	3.3E-21	2.0E-16	0.
PROPYNE	2.7E-27	4.7E-25	7.9E-17	3.2E-30	2.9E-23	7.0E-17	0.
BUTYNE	4.9E-33	4.5E-30	2.8E-20	1.9E-36	1.1E-27	1.1E-19	0.
OCTYNE	0.	0.	1.7E-33	0.	0.	4.3E-32	0.
ALLENE	3.3E-28	5.6E-26	3.5E-18	3.8E-31	3.5E-24	8.4E-18	0.
TOLUENE	5.8E-31	1.0E-25	2.5E-06	8.9E-39	1.5E-21	1.4E-05	0.
XYLENE	4.8E-36	4.6E-30	1.1E-08	0.	2.7E-25	9.4E-08	0.
BIPHENYL	0.	0.	1.5E-07	0.	5.0E-37	1.0E-06	0.
ANTHACENE	0.	0.	2.1E-06	0.	0.	1.3E-05	0.
FURAN	1.9E-30	1.1E-27	6.5E-18	4.2E-37	7.8E-26	9.1E-18	0.
PHENOL	3.7E-32	6.9E-28	2.5E-12	0.	7.4E-25	5.3E-12	0.
BENZOIC ACID	1.9E-33	1.2E-28	4.2E-11	0.	1.5E-25	5.1E-11	0.
METHANOL	1.0E-12	2.6E-12	6.4E-14	1.6E-13	3.4E-12	1.1E-13	0.
ETHANOL	3.2E-17	4.4E-16	1.1E-15	1.7E-18	2.3E-15	2.8E-15	0.
OCTANOL	0.	0.	8.9E-36	0.	0.	4.0E-34	0.
GLYCOL	2.0E-26	1.5E-25	5.4E-27	1.7E-29	2.3E-25	8.9E-27	0.
GLYCHROL	0.	0.	0.	0.	0.	0.	0.
FORMALDEHYDE	4.0E-13	1.2E-12	1.8E-12	2.2E-15	1.4E-12	1.7E-12	0.
ACETALDEHYDE	1.1E-15	1.8E-14	2.7E-12	2.0E-18	8.7E-14	4.2E-12	0.
GLYCAL	1.4E-23	1.4E-22	2.0E-20	1.5E-29	1.9E-22	1.2E-20	0.
GLYCOLALDEHYDE	1.2E-24	1.0E-23	2.3E-23	3.5E-29	1.5E-23	2.3E-23	0.
GLYCERALDEHYDE	0.	5.4E-38	1.9E-37	0.	9.6E-38	1.8E-37	0.
FORMIC ACID	1.4E-10	2.2E-10	5.1E-12	1.2E-14	7.9E-11	3.1E-12	1.1E-31
ACETIC ACID	1.7E-11	1.4E-10	3.3E-10	5.0E-16	2.1E-10	3.2E-10	0.
PROPIONIC ACID	1.6E-17	7.1E-16	1.6E-13	1.5E-22	4.3E-15	2.5E-13	0.
BUTYRIC ACID	1.5E-23	3.6E-21	8.2E-17	4.6E-29	8.7E-20	2.0E-16	0.
OCTANIC ACID	0.	0.	1.1E-29	0.	3.2E-38	1.8E-28	0.
NONANIC ACID	0.	0.	2.6E-33	0.	0.	6.7E-32	0.
PROPENIC ACID	9.0E-21	4.7E-19	6.8E-15	3.0E-27	2.6E-18	6.2E-15	0.
GLYXALIC ACID	1.9E-18	1.0E-17	2.3E-17	3.3E-26	4.3E-18	8.1E-18	0.
OXALIC ACID	6.3E-14	1.9E-13	6.3E-15	1.8E-23	2.3E-14	1.4E-15	4.7E-35
GLYCOLIC ACID	3.6E-20	1.7E-19	6.0E-21	1.8E-26	7.5E-20	3.6E-21	0.
PYRUVIC ACID	1.0E-33	2.9E-32	6.3E-30	0.	4.8E-32	3.5E-30	0.
LACTIC ACID	3.0E-26	7.5E-25	2.6E-24	4.9E-33	1.3E-24	2.5E-24	0.
GLYCERIC ACID	5.8E-35	8.0E-34	4.3E-35	0.	4.3E-34	2.5E-35	0.
FUMARIC ACID	1.4E-29	1.3E-27	2.8E-23	0.	2.5E-27	9.1E-24	0.
CROTONIC ACID	7.5E-27	2.1E-24	3.0E-18	8.1E-34	4.7E-23	4.4E-18	0.
ACETOACET. ACID	1.5E-28	2.3E-26	5.1E-22	2.8E-37	1.6E-25	4.6E-22	0.
OXALOACET. ACID	2.1E-31	1.1E-29	3.6E-27	0.	6.3E-30	7.2E-28	0.
Α-KETCHUT. ACID	1.2E-28	1.8E-26	3.9E-22	2.1E-37	1.2E-25	3.5E-22	0.
ACETOXYAC. ACID	0.	5.6E-39	1.9E-36	0.	1.1E-38	1.0E-36	0.
SUCCINIC ACID	2.8E-26	2.3E-24	7.7E-22	8.3E-37	4.7E-24	4.3E-22	0.
OHBUTYRIC ACID	2.9E-32	3.8E-30	1.3E-27	0.	2.8E-29	2.0E-27	0.
METHYLACETATE	3.8E-32	1.7E-30	4.0E-28	3.6E-37	1.0E-29	6.1E-28	0.
ETHYLACETATE	4.0E-38	9.5E-36	2.2E-31	0.	2.3E-34	5.4E-31	0.
ACETICANHYDRIDE	0.	0.	7.2E-37	0.	0.	6.5E-37	0.
ETHYLENE OXIDE	5.3E-29	8.2E-28	1.2E-25	9.4E-32	4.1E-27	2.0E-25	0.
PROPYLENE OXIDE	1.1E-32	9.4E-31	1.4E-26	6.6E-36	1.9E-29	3.6E-26	0.
ACETONE	6.0E-19	5.0E-17	7.5E-13	3.5E-22	1.0E-15	1.9E-12	0.
DIMETHYL ETHER	2.0E-21	2.7E-20	6.4E-20	1.0E-22	1.4E-19	1.7E-19	0.
KETENE	5.5E-19	9.8E-18	9.3E-14	3.3E-23	4.5E-17	8.6E-14	0.
RIBOSE	0.	0.	0.	0.	0.	0.	0.

AT C•2 ATM AND 500.0C KÉLVIN

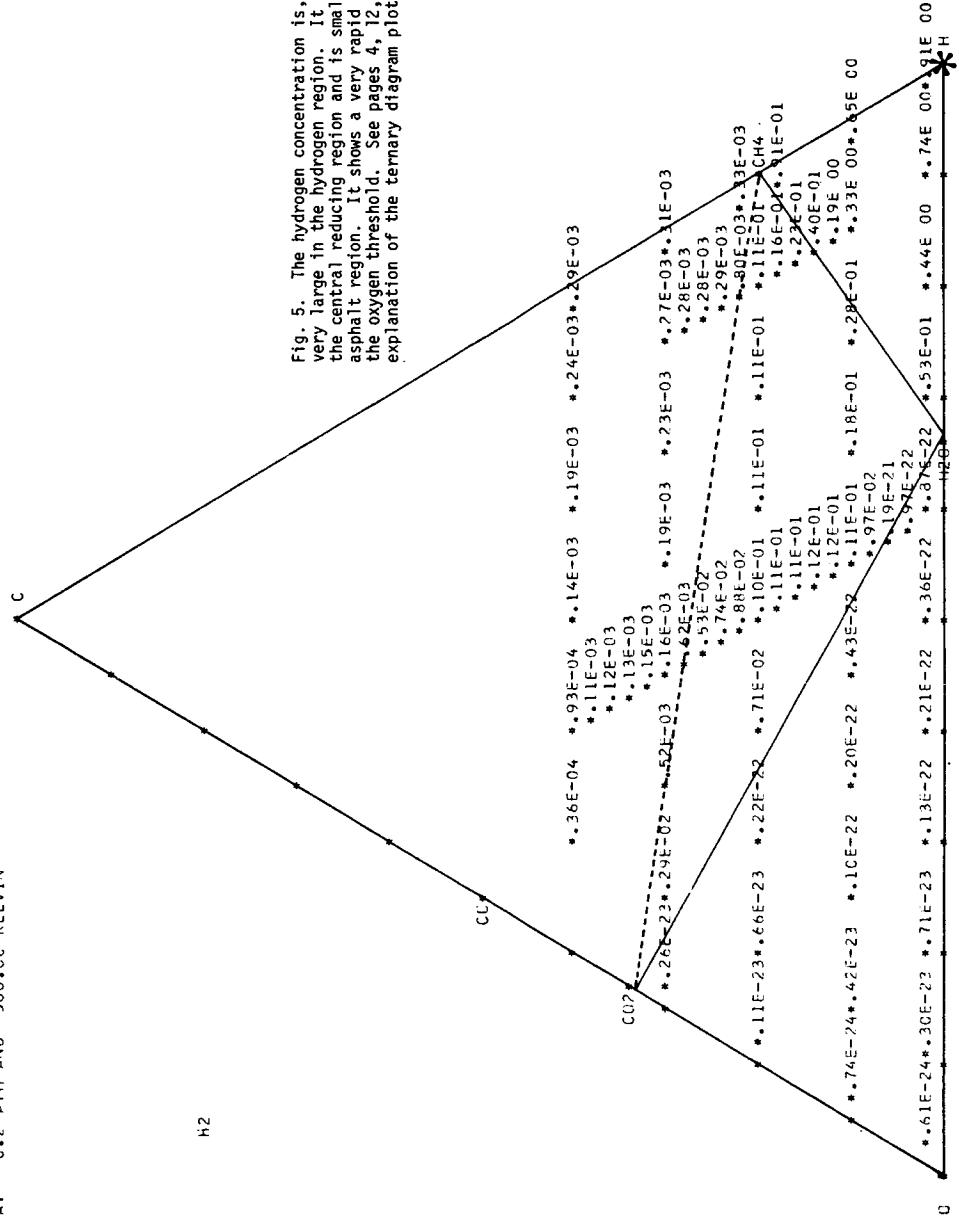
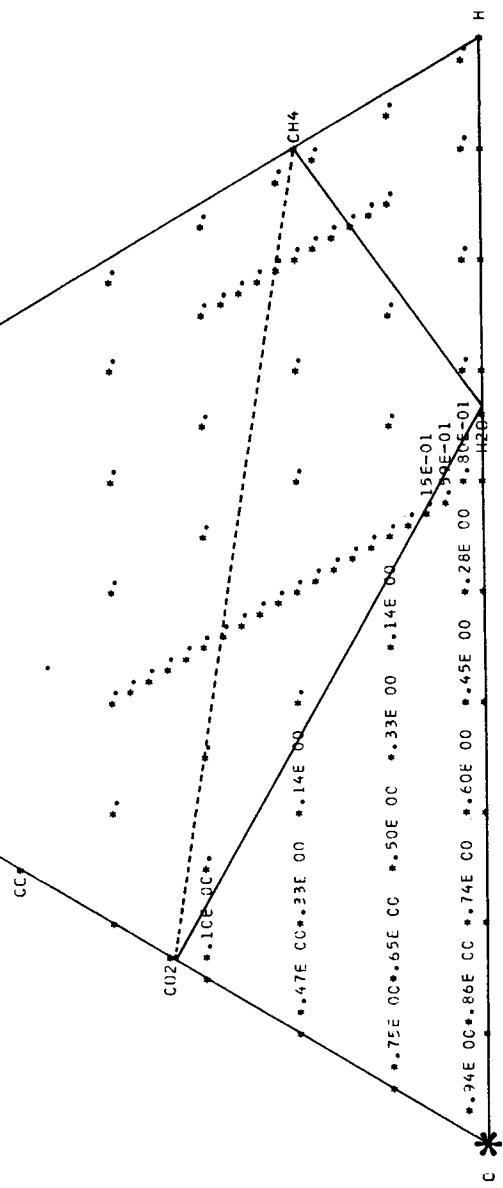


Fig. 5. The hydrogen concentration is, as expected, very large in the hydrogen region. It is smaller in the central reducing region and is smaller yet in the asphalt region. It shows a very rapid decrease across the oxygen threshold. See pages 4, 12, and 16 for an explanation of the ternary diagram plots.

AT C\*2 AT\* AND 5CO\*OC KELVIN

02

Fig. 6. The oxygen concentration is high only in the oxygen region and negligible everywhere else.



AT C.2 ATM AND 500.00 KELVIN

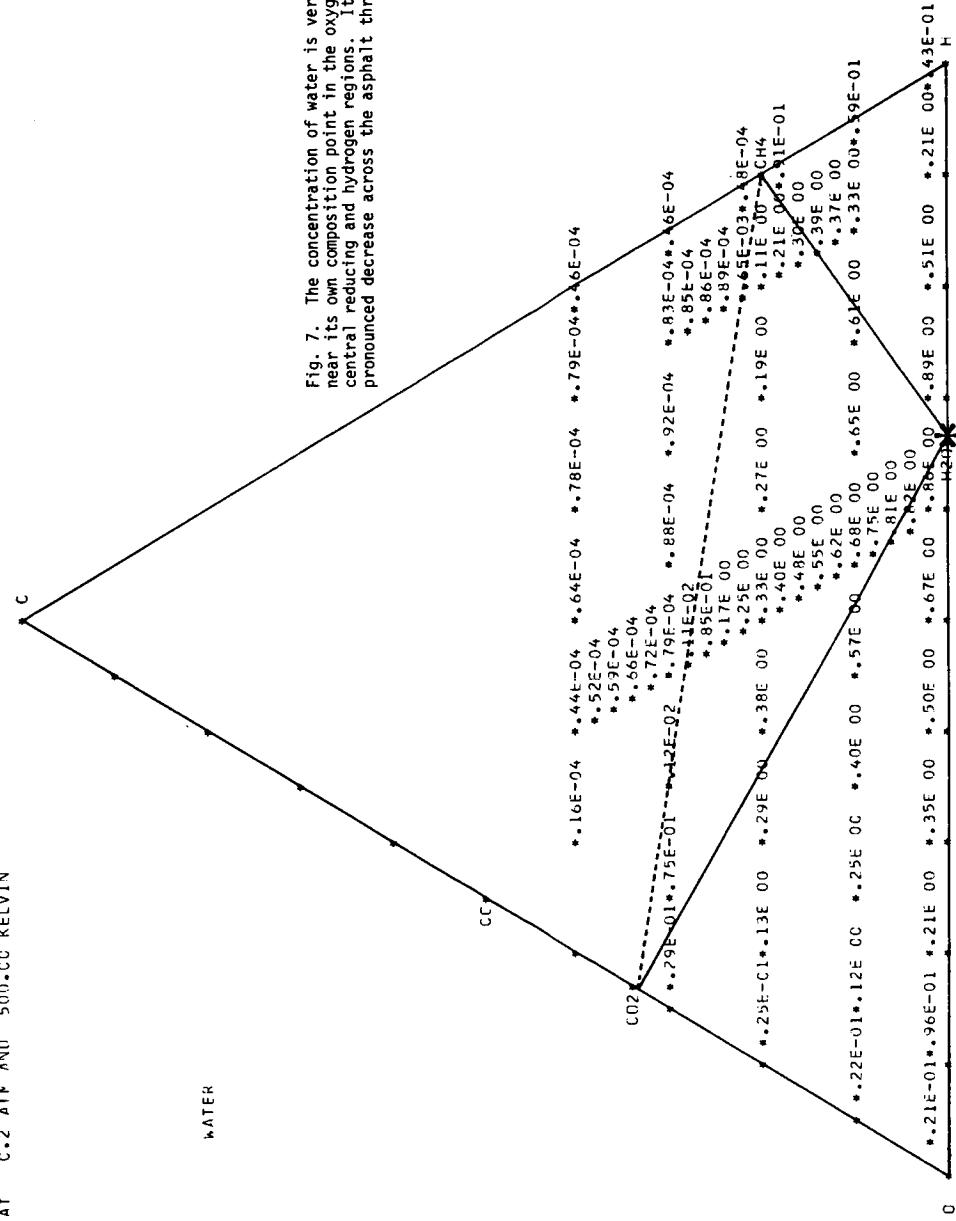


Fig. 7. The concentration of water is very large near its own composition point in the oxygen, central reducing and hydrogen regions. It shows a pronounced decrease across the asphalt threshold.

AT C=2 ATM AND 500.0C KELVIN

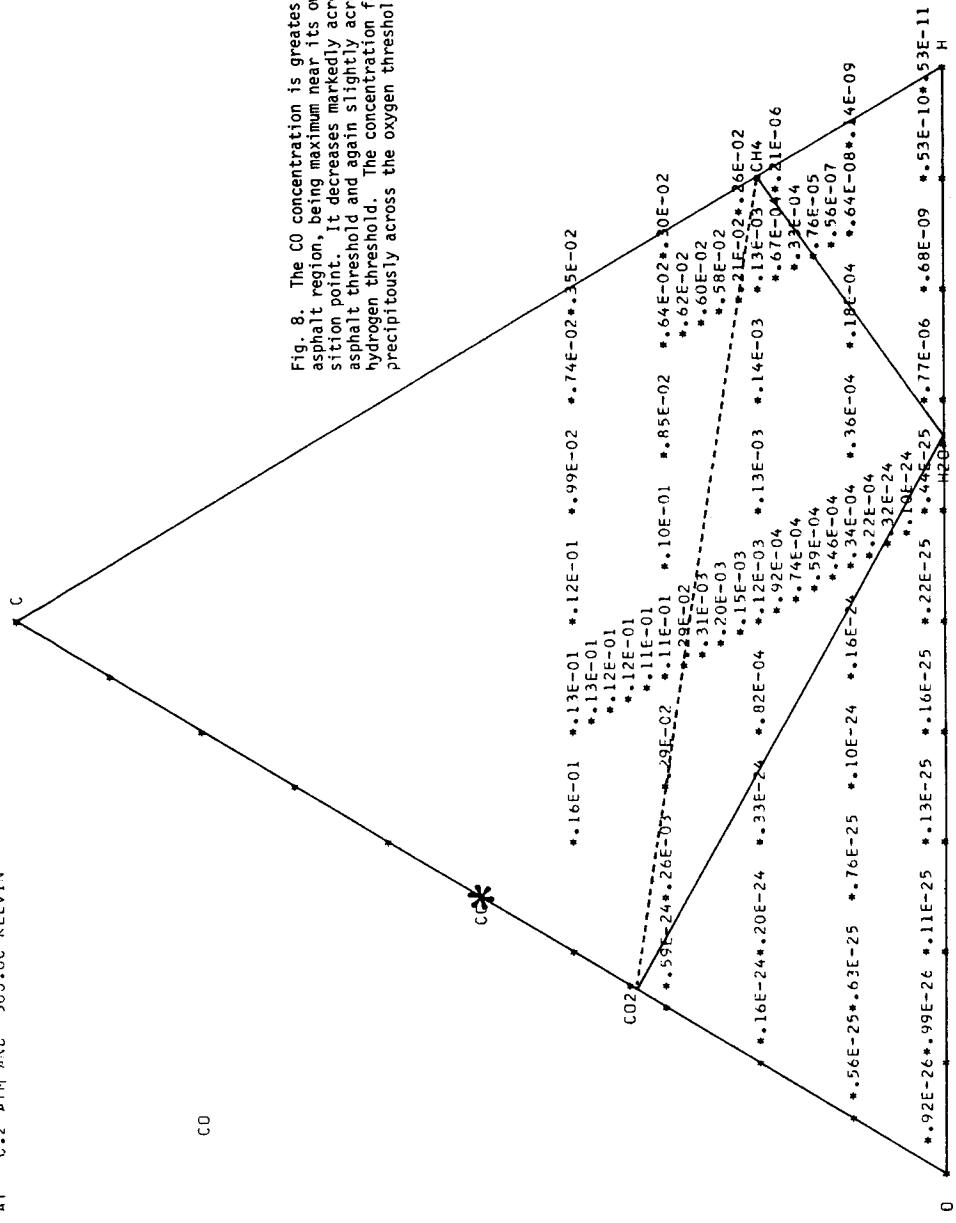
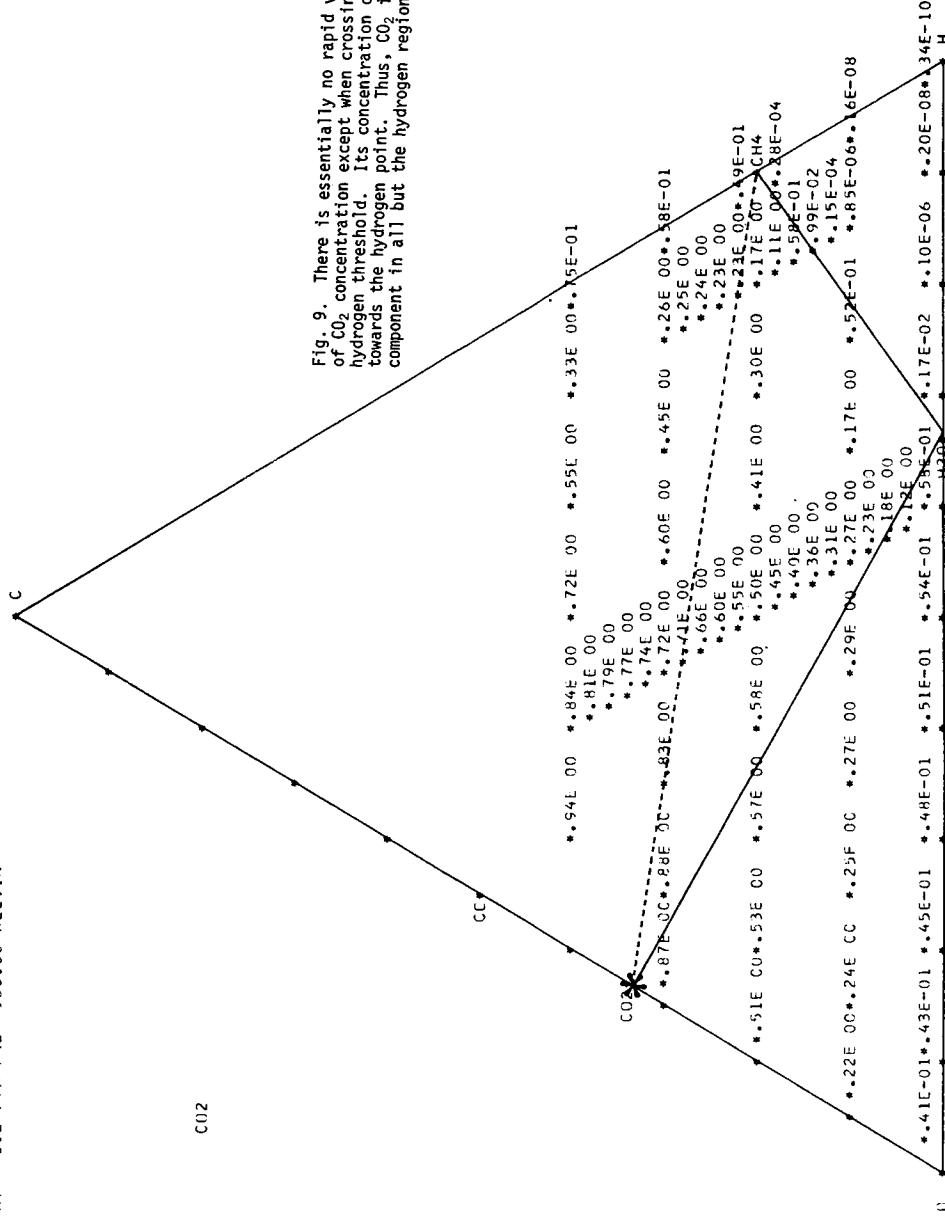


Fig. 8. The CO concentration is greatest in the asphalt region, being maximum near its own composition point. It decreases markedly across the asphalt threshold and again slightly across the hydrogen threshold. The concentration falls off precipitously across the oxygen threshold.



**Fig. 9.** There is essentially no rapid variation of CO<sub>2</sub> concentration except when crossing the hydrogen threshold. Its concentration decreases towards the hydrogen point. Thus, CO<sub>2</sub> is a major component in all but the hydrogen region.

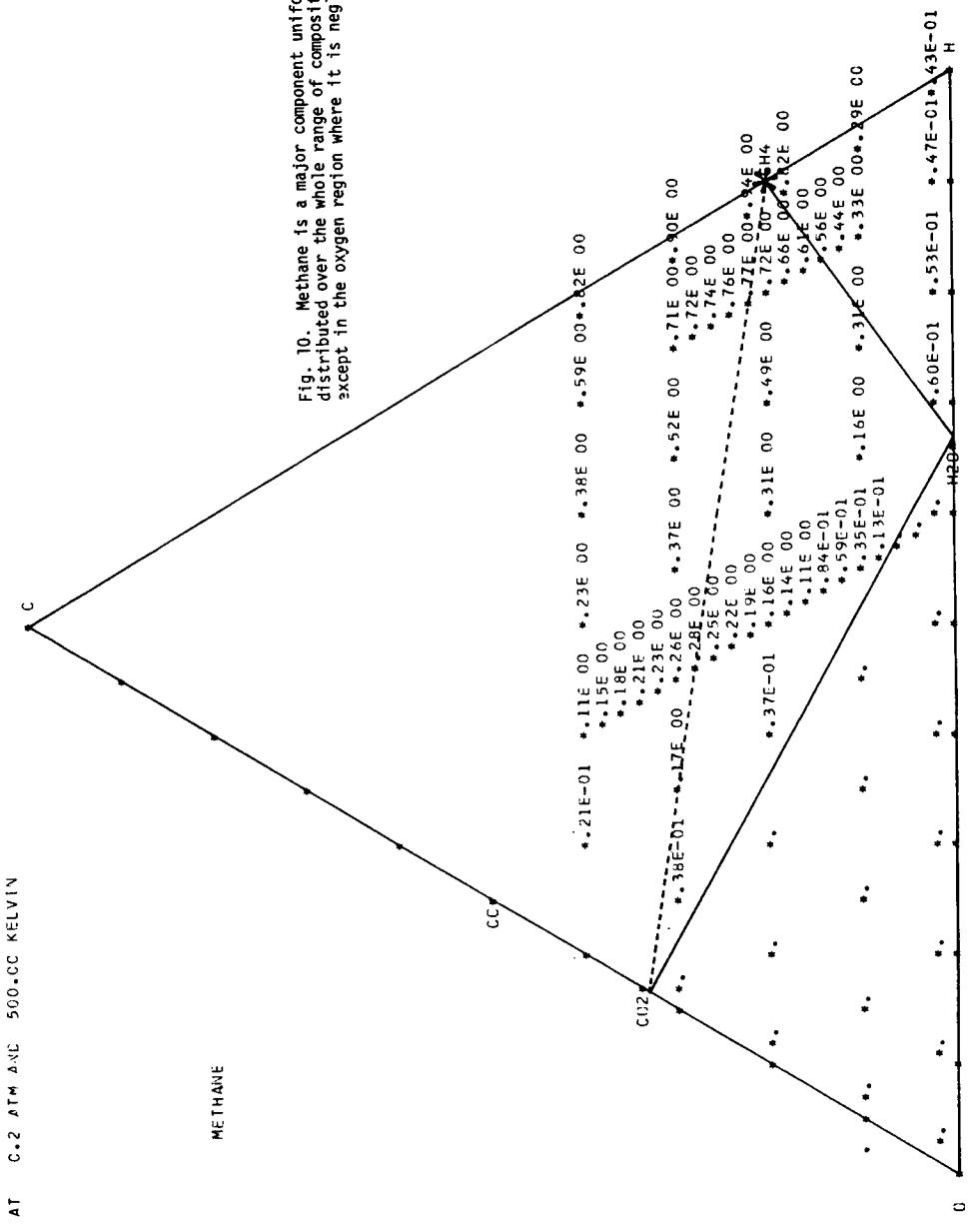


Fig. 10. Methane is a major component uniformly distributed over the whole range of compositions except in the oxygen region where it is negligible.

AT C.2 AIM AND 500.00 KELVIN

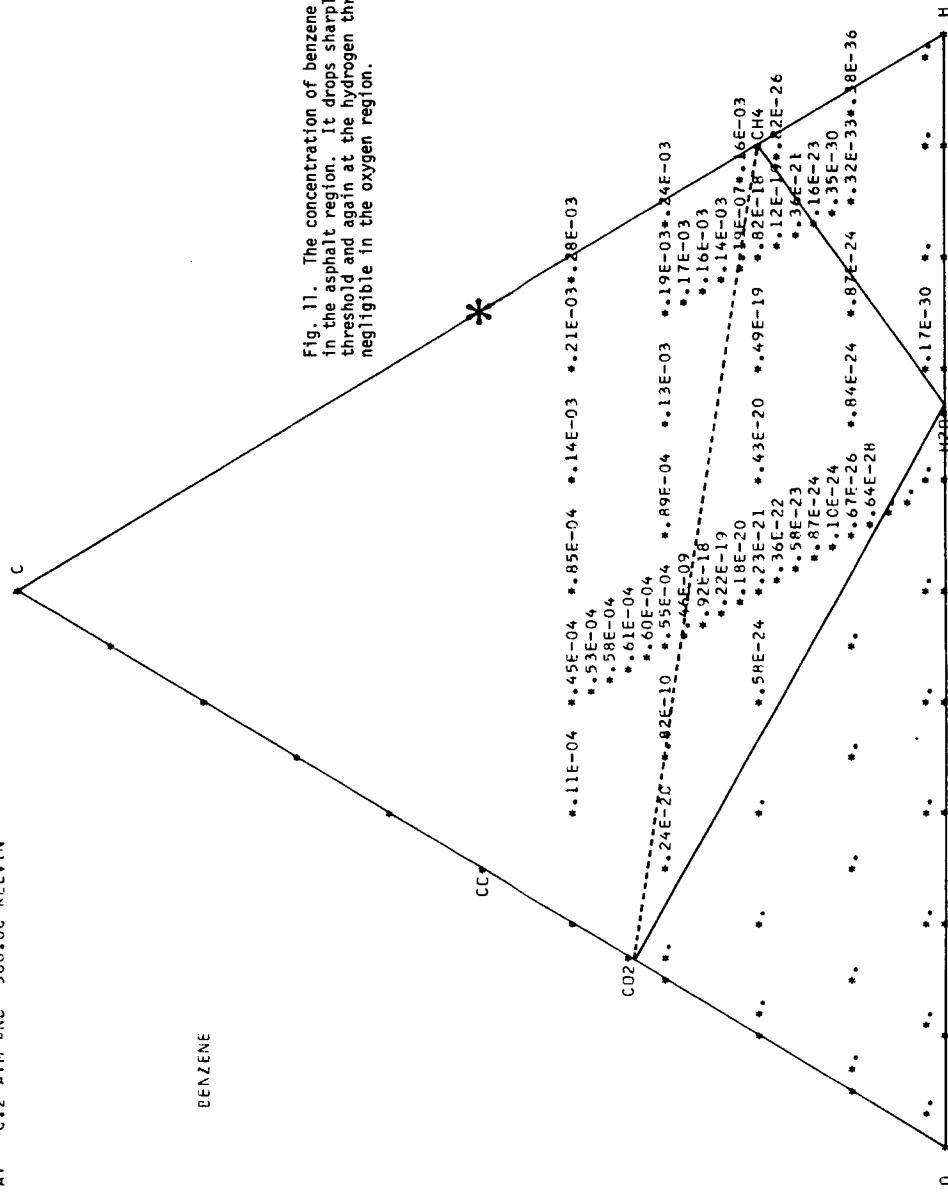


Fig. 11. The concentration of benzene is large only in the asphalt region. It drops sharply at the asphalt threshold and again at the hydrogen threshold. It is negligible in the oxygen region.

ATM C.2 ATM AND 500.00 KELVIN

NAPHTHALENE

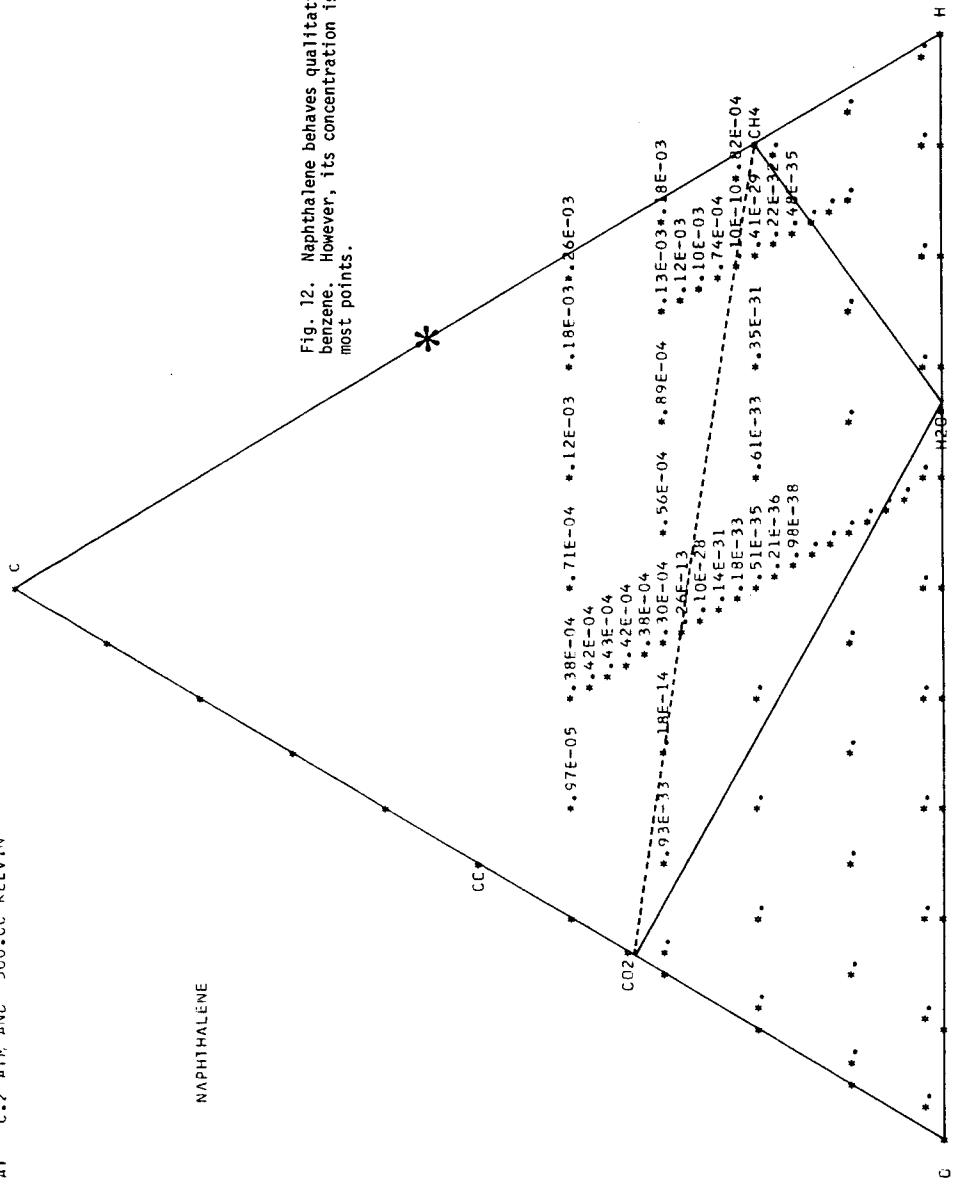


Fig. 12. Naphthalene behaves qualitatively like benzene. However, its concentration is lower at most points.

AT C=2 ATM ANL 500.00 KELVIN

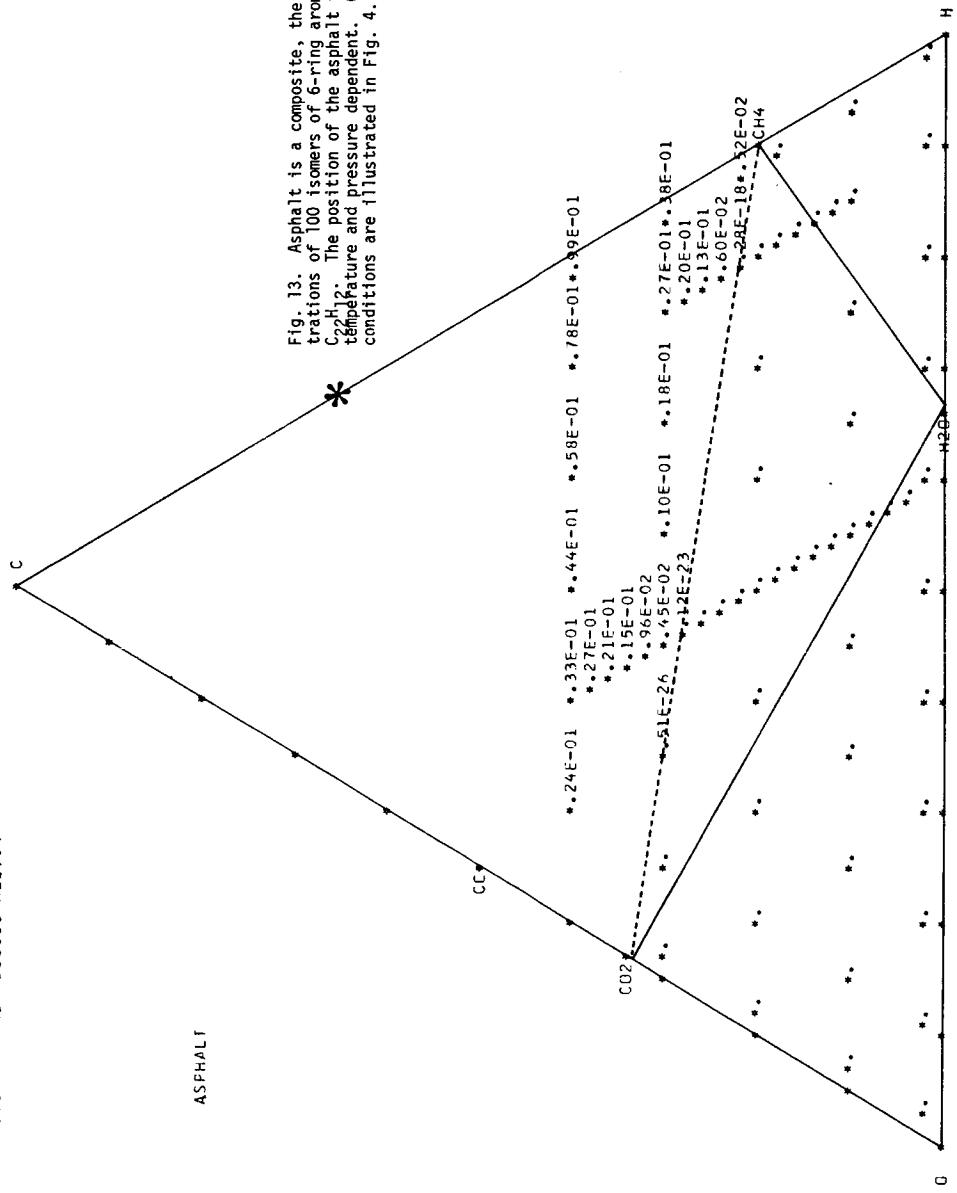


Fig. 13. Asphalt is a composite, the sum of concentrations of 100 isomers of 6-ring aromatic compounds, C<sub>22</sub>H<sub>22</sub>. The position of the asphalt threshold is temperature and pressure dependent. Curves for other conditions are illustrated in Fig. 4.

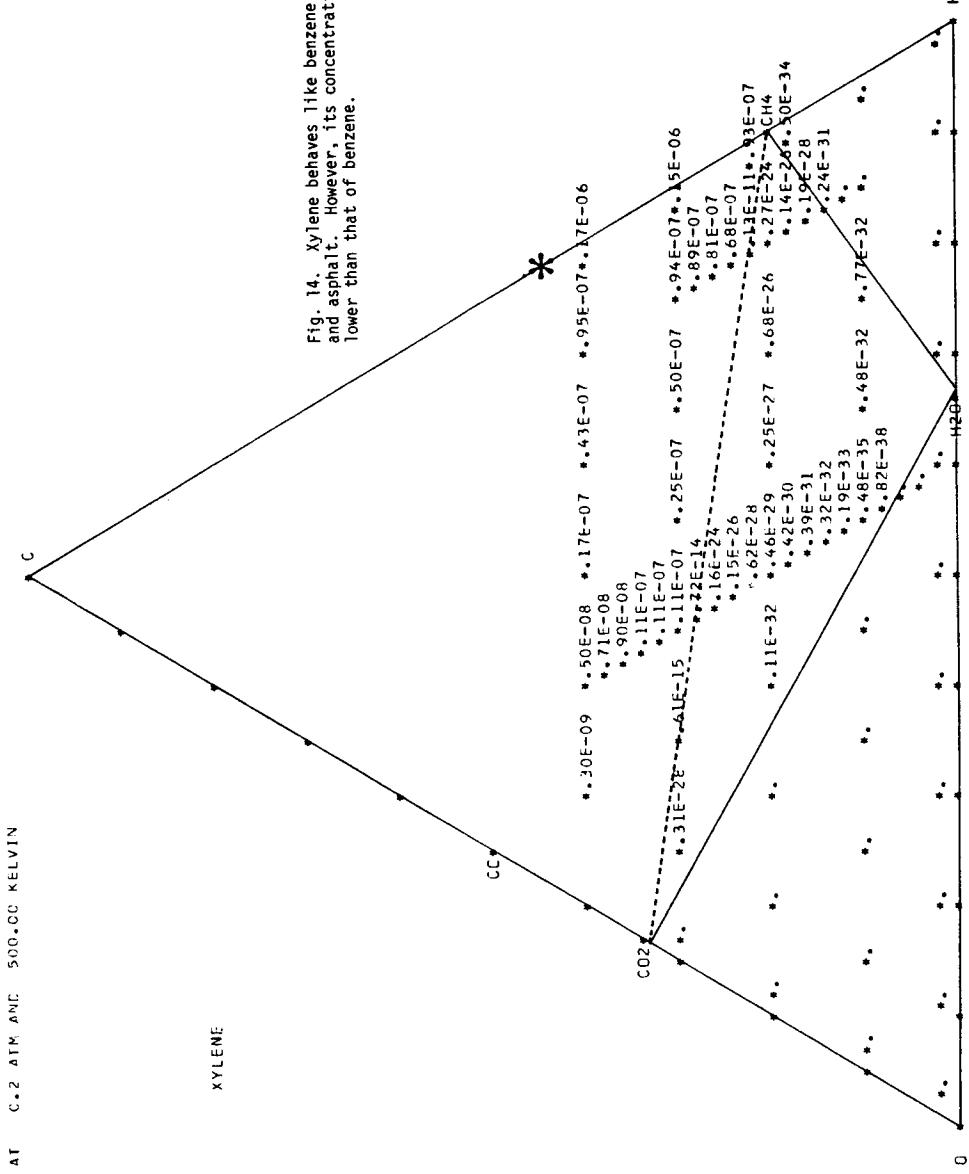
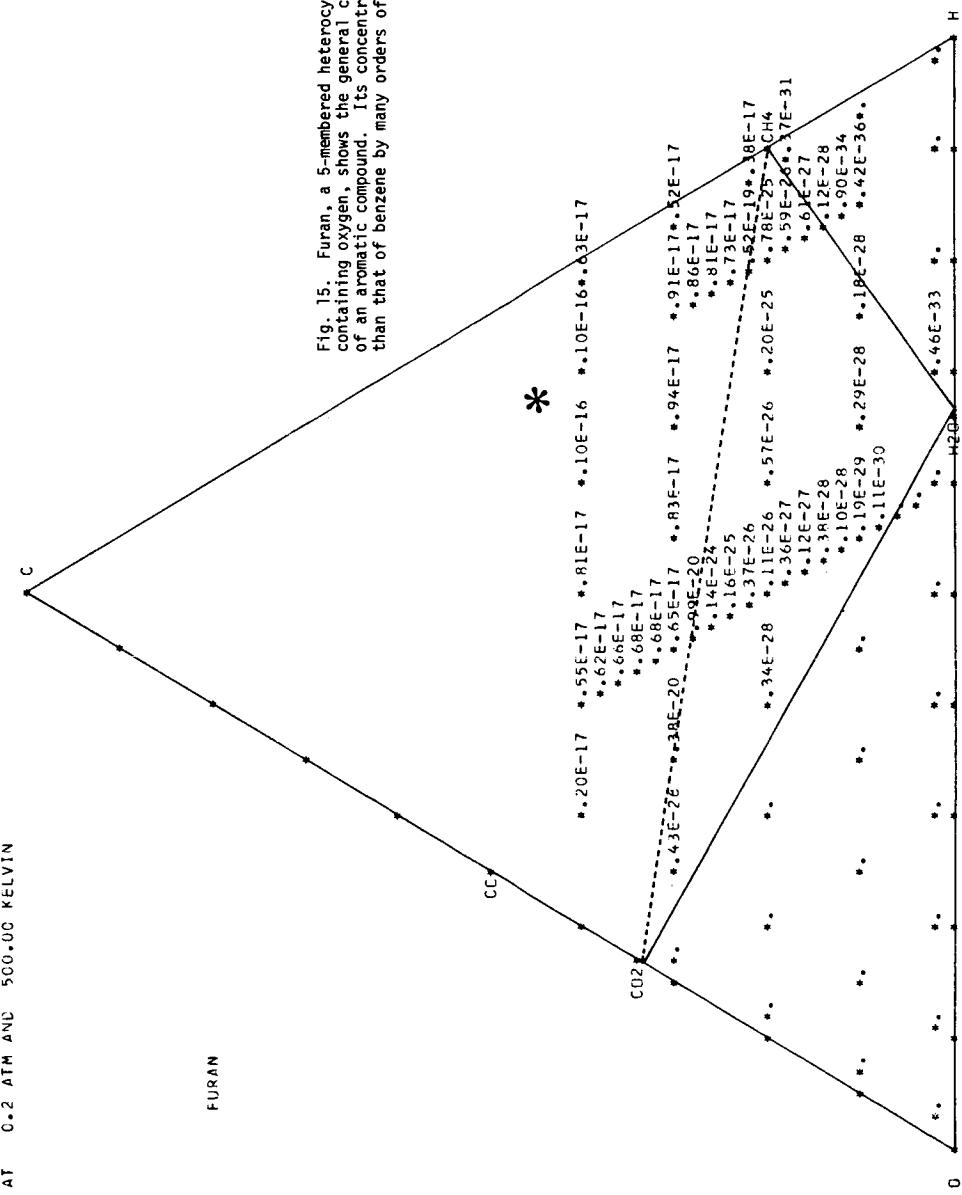


Fig. 14. Xylene behaves like benzene, naphthalene, and asphalt. However, its concentration is much lower than that of benzene.

AT 0.2 ATM AND 500.00 KELVIN



AT C.2 ATM AND 500.00 KELVIN

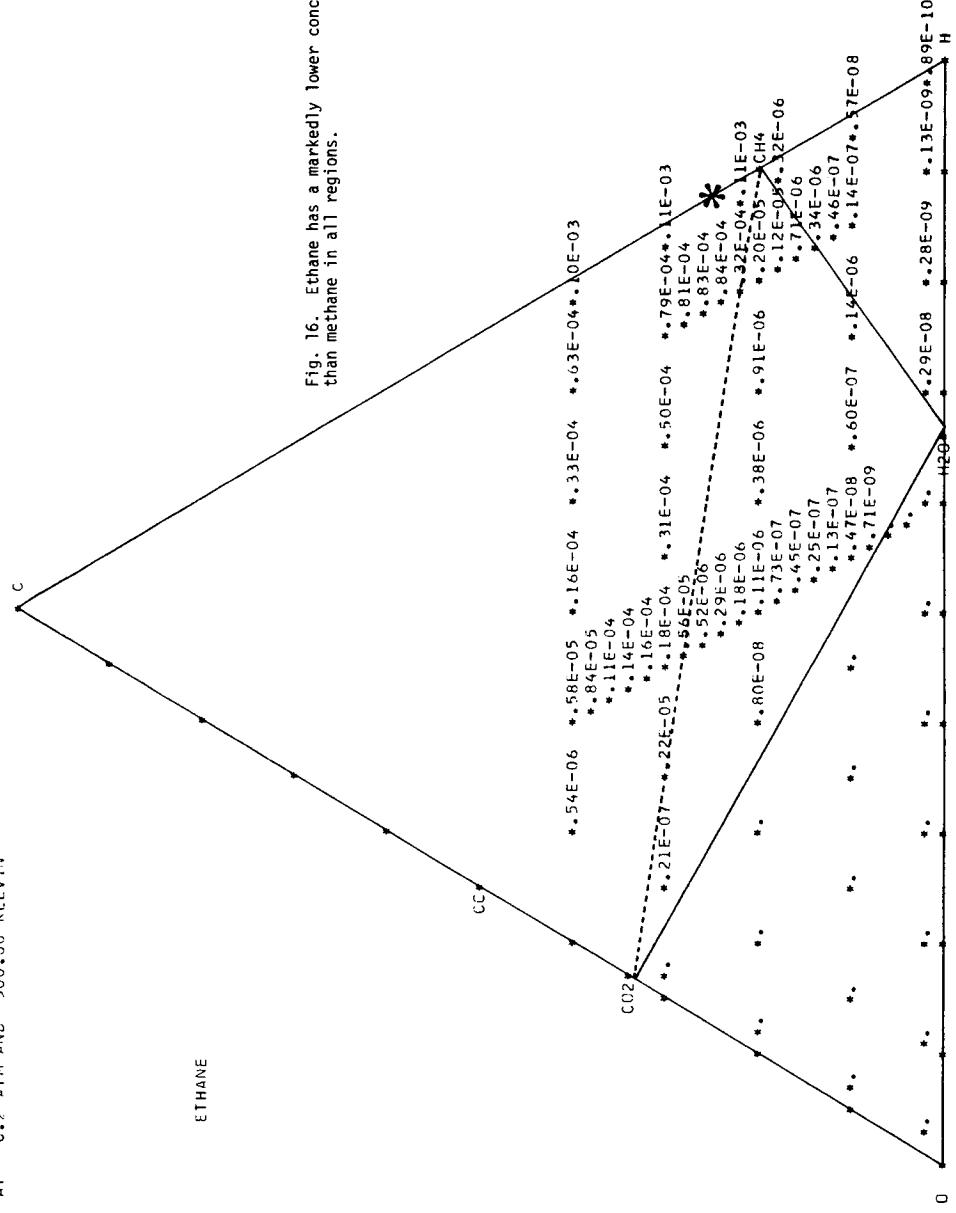
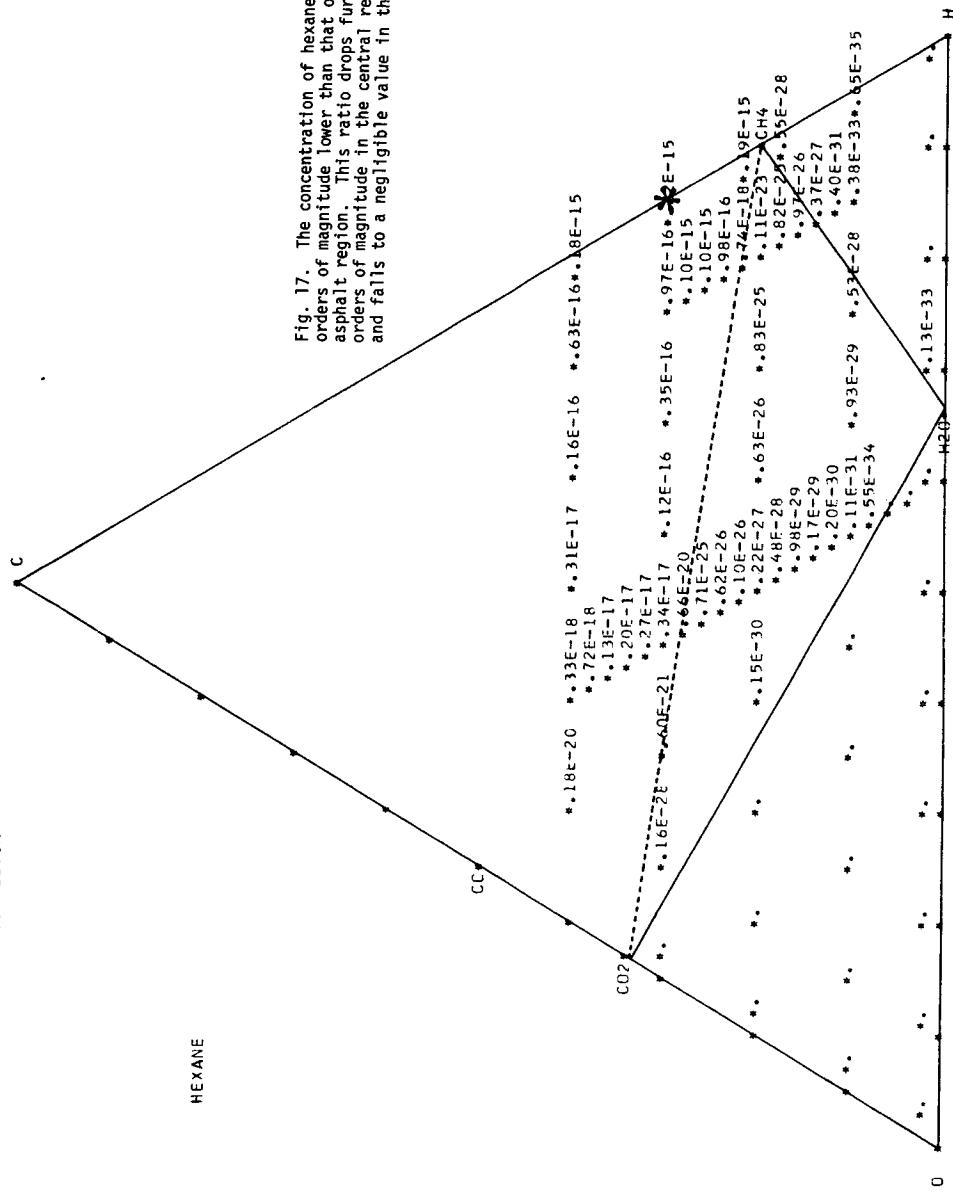


Fig. 16. Ethane has a markedly lower concentration than methane in all regions.

AT C\*2 ATM ANC 500\*CC KELVIN



$\Delta T$  C.2 ATM AND 500.0°C KELVIN

CYCLOHEXANE

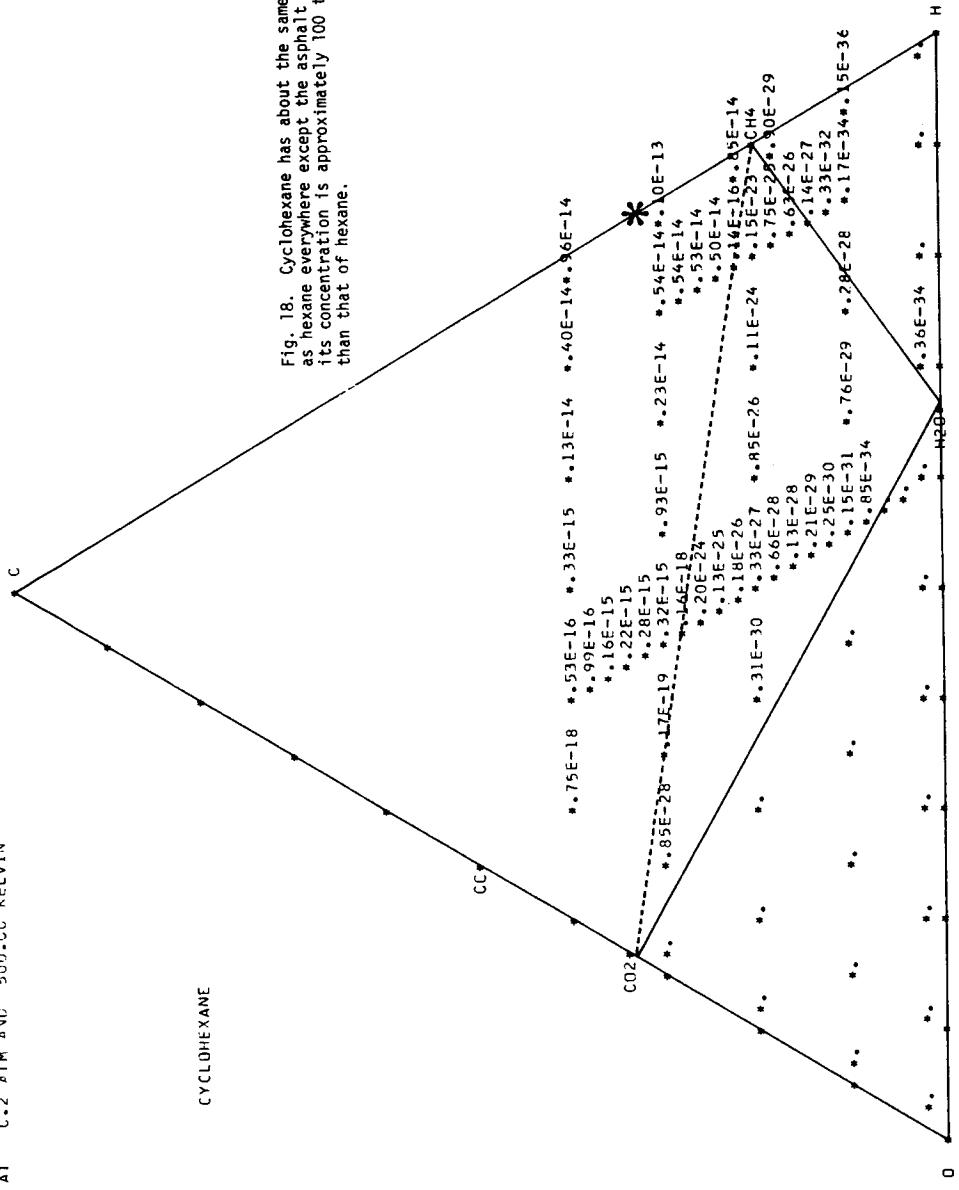


Fig. 18. Cyclohexane has about the same concentration as hexane everywhere except the asphalt region. Here its concentration is approximately 100 times higher than that of hexane.

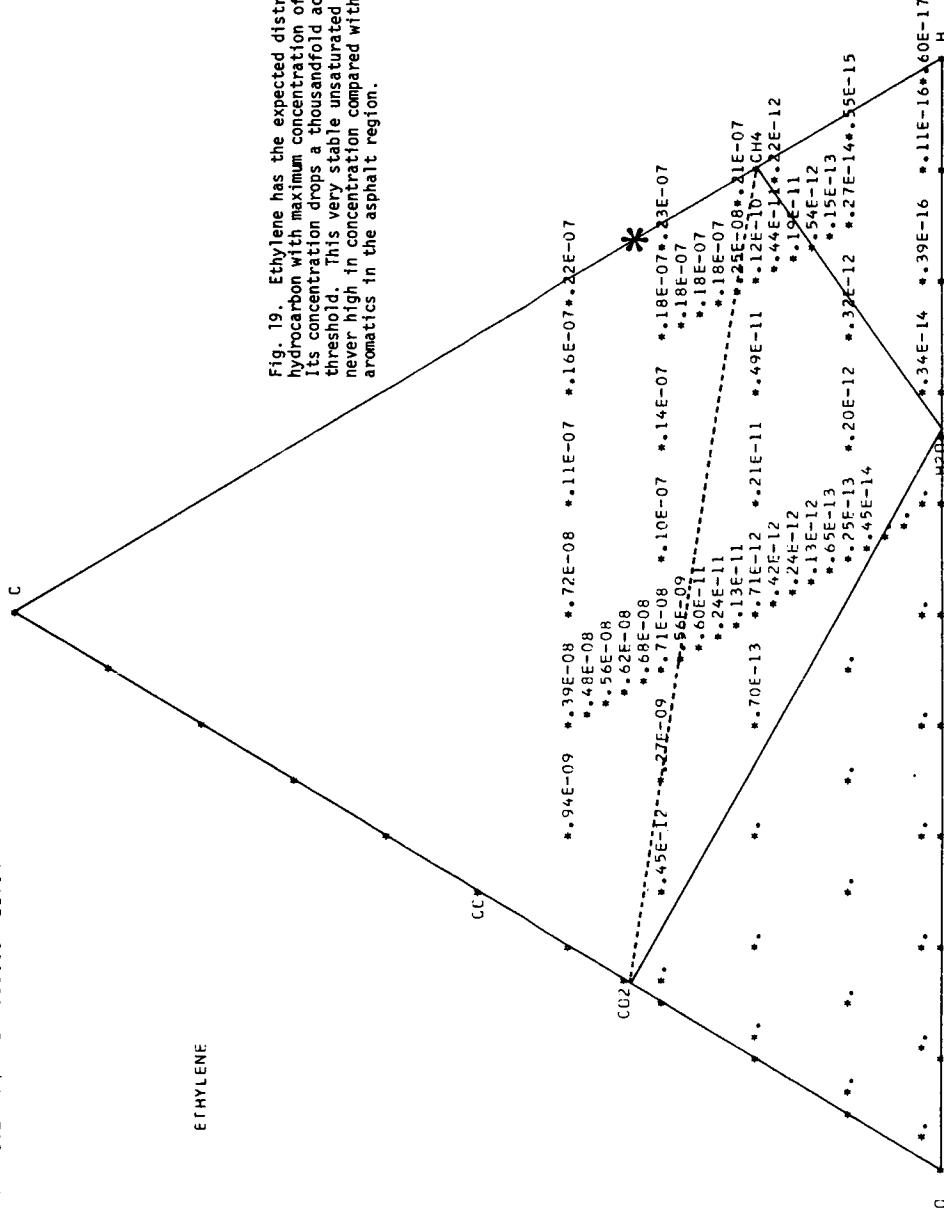


Fig. 19. Ethylene has the expected distribution of a hydrocarbon with maximum concentration of about  $10^{-7}$ . Its concentration drops a thousandfold across the asphalt threshold. This very stable unsaturated hydrocarbon is never high in concentration compared with methane or with aromatics in the asphalt region.

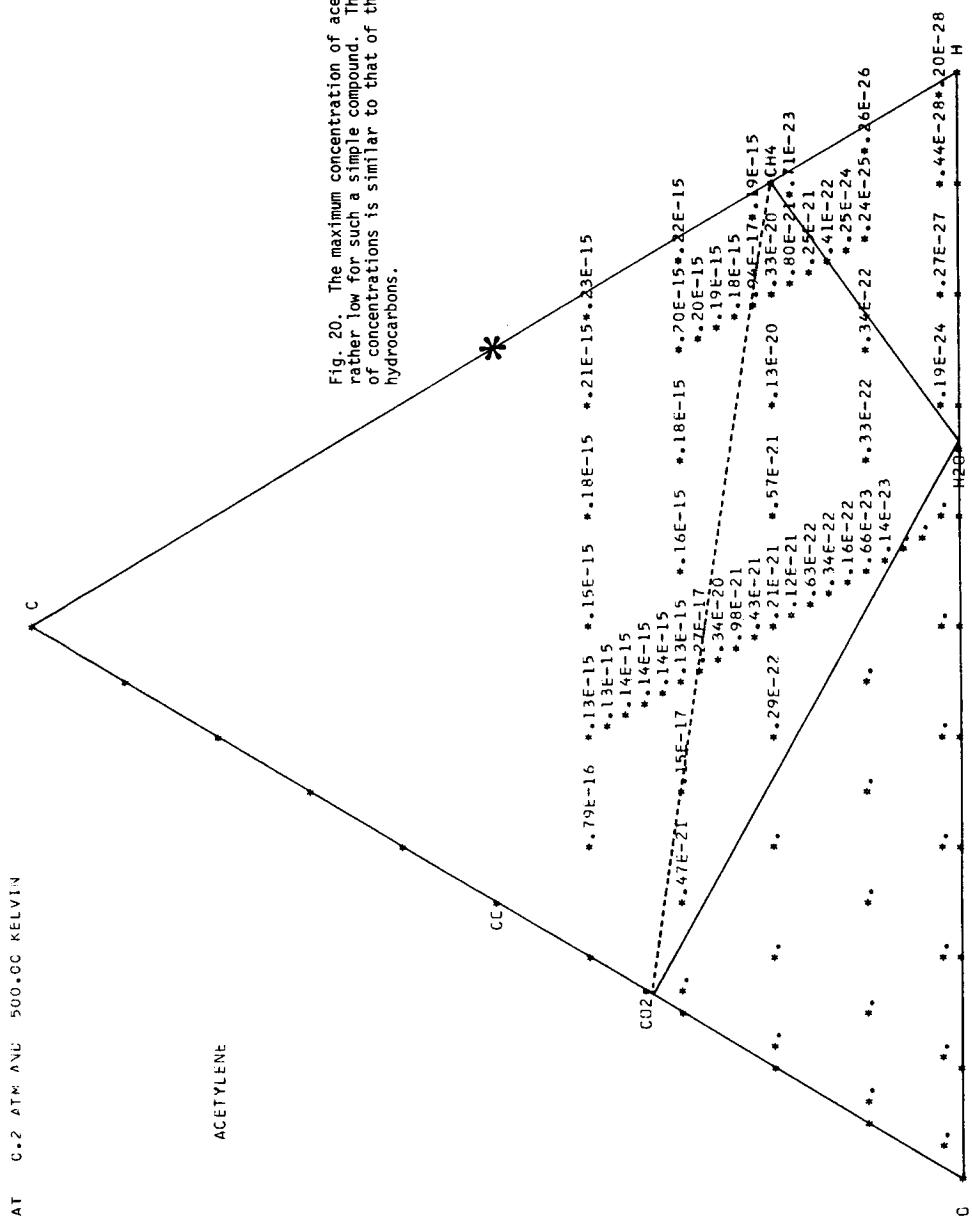


Fig. 20. The maximum concentration of acetylene is rather low for such a simple compound. The pattern of concentrations is similar to that of the saturated hydrocarbons.

AT 0.2 ATM AND 500.00 KELVIN

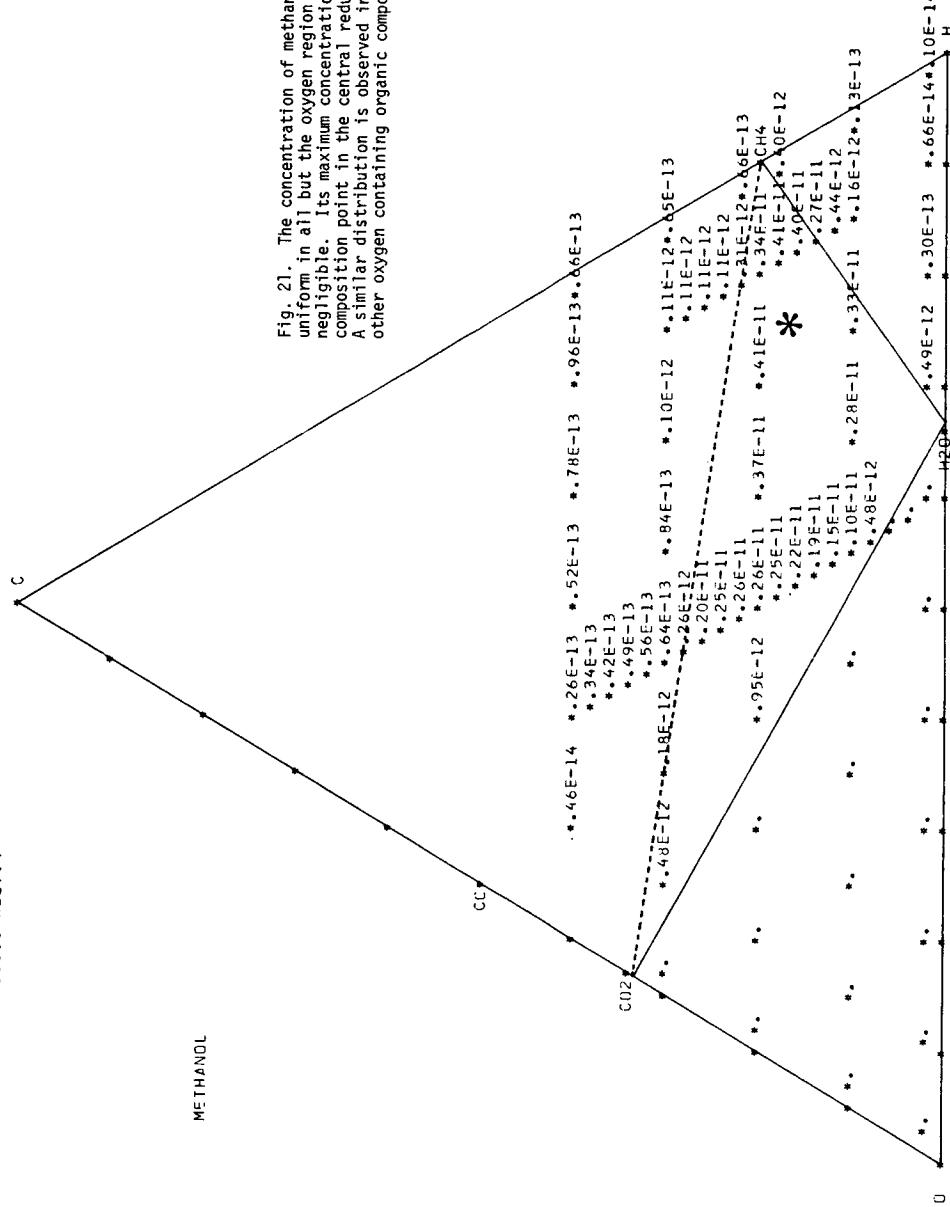


Fig. 21. The concentration of methanol is rather uniform in all but the oxygen region where it is negligible. Its maximum concentration is near its composition point in the central reducing region. A similar distribution is observed in a number of other oxygen containing organic compounds.

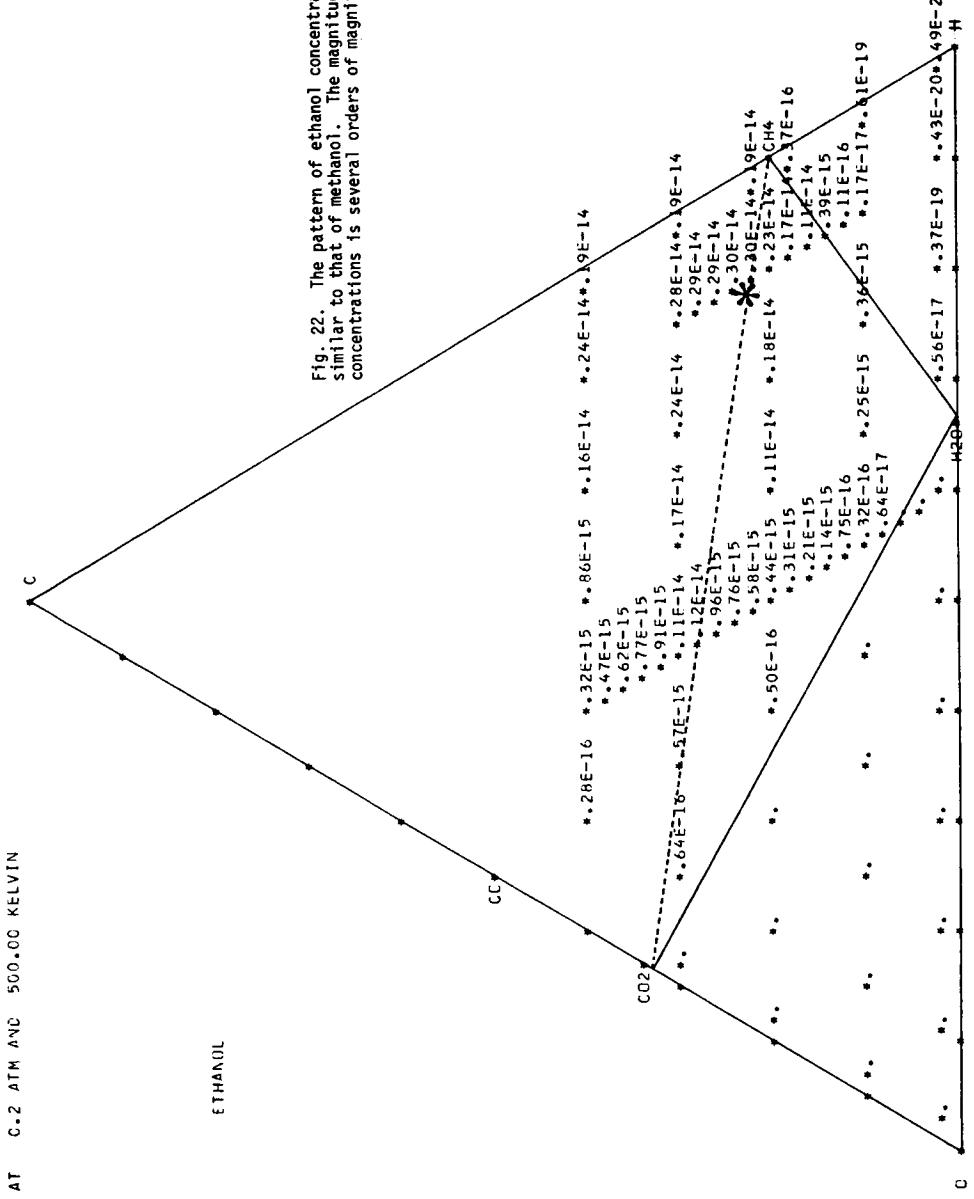


Fig. 22. The pattern of ethanol concentrations is similar to that of methanol. The magnitude of the concentrations is several orders of magnitude smaller.

AT 0.2 ATM AND 500.00 KELVIN

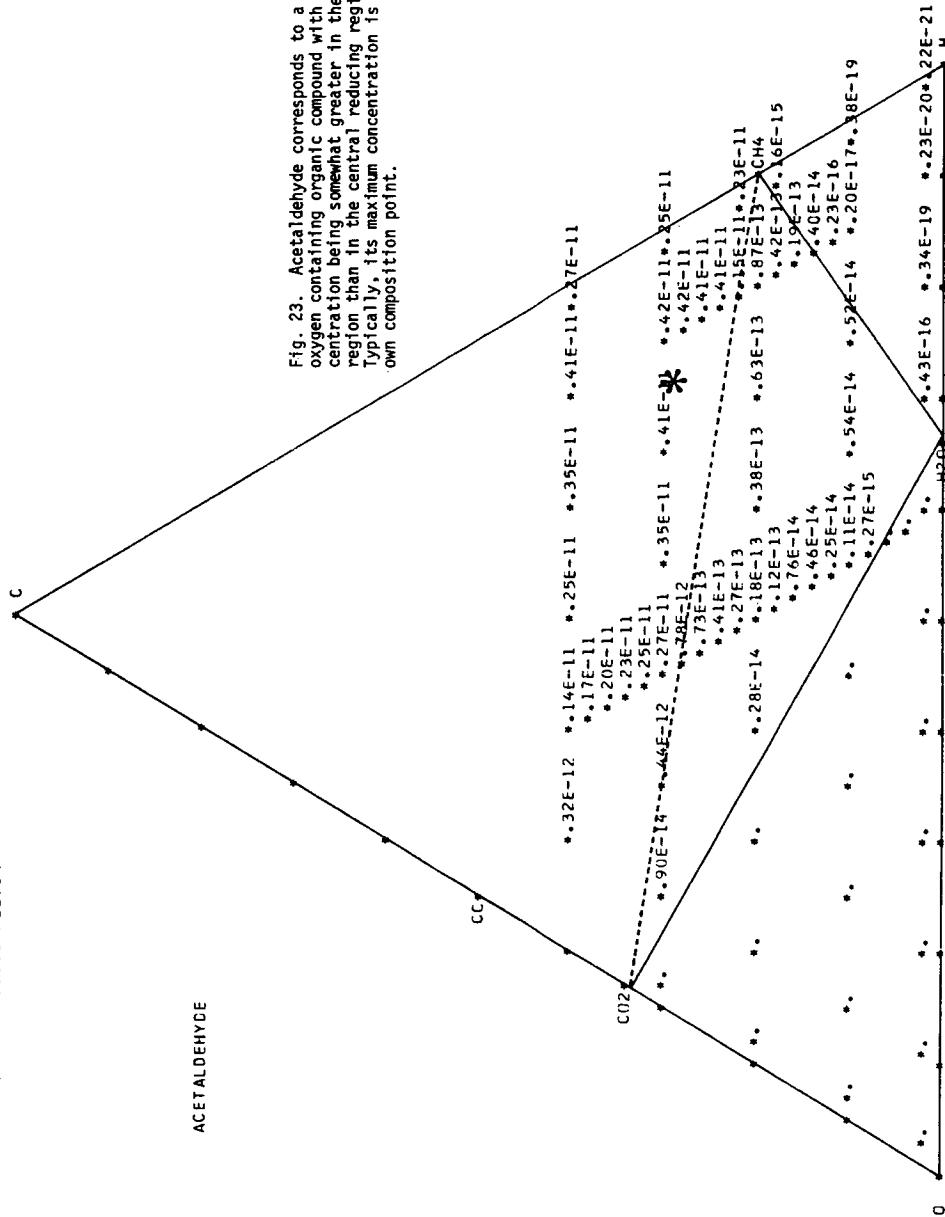


Fig. 23. Acetaldehyde corresponds to a typical oxygen containing organic compound with the concentration being somewhat greater in the asphalt region than in the central reducing region. Typically, its maximum concentration is near its own composition point.

AT C=2 ATM AND 560.0°C KELVIN

C

FORMIC ACID

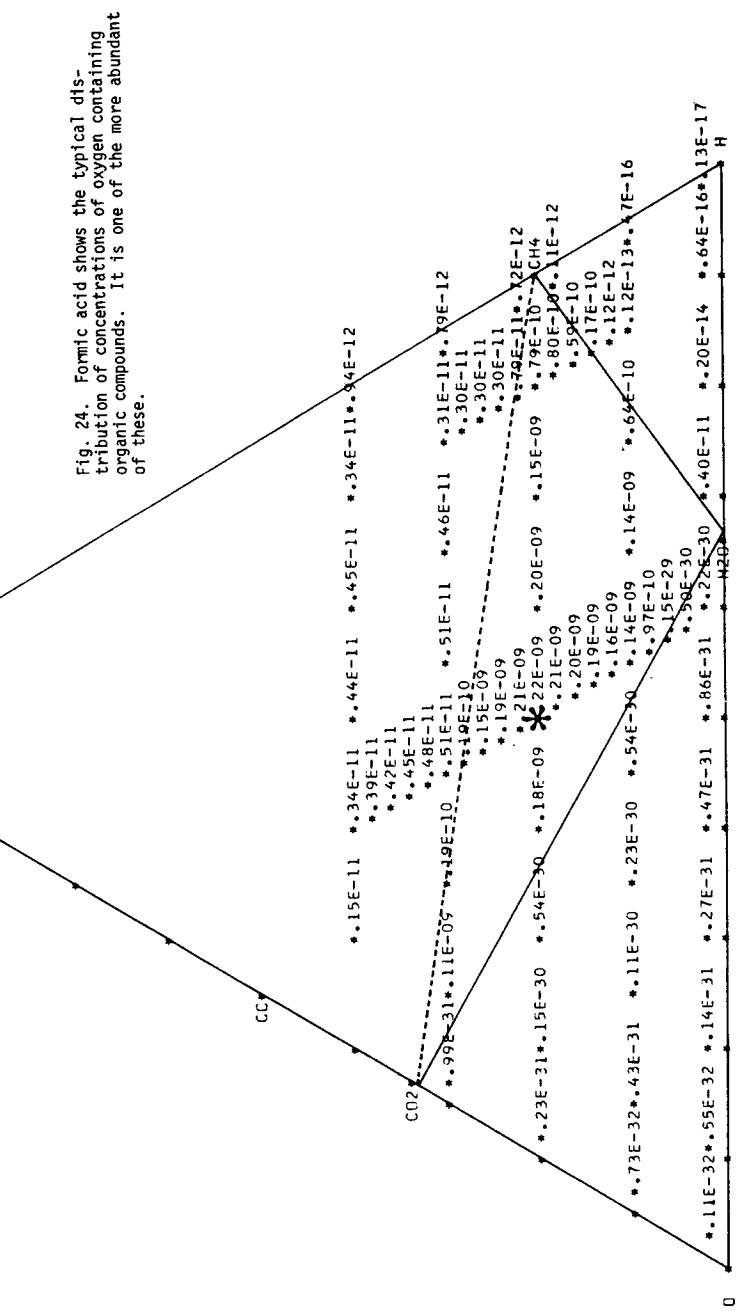


Fig. 24. Formic acid shows the typical distribution of concentrations of oxygen containing organic compounds. It is one of the more abundant of these.

ATM 0.2 ATM AND 500.0°C KELVIN

ACETIC ACID

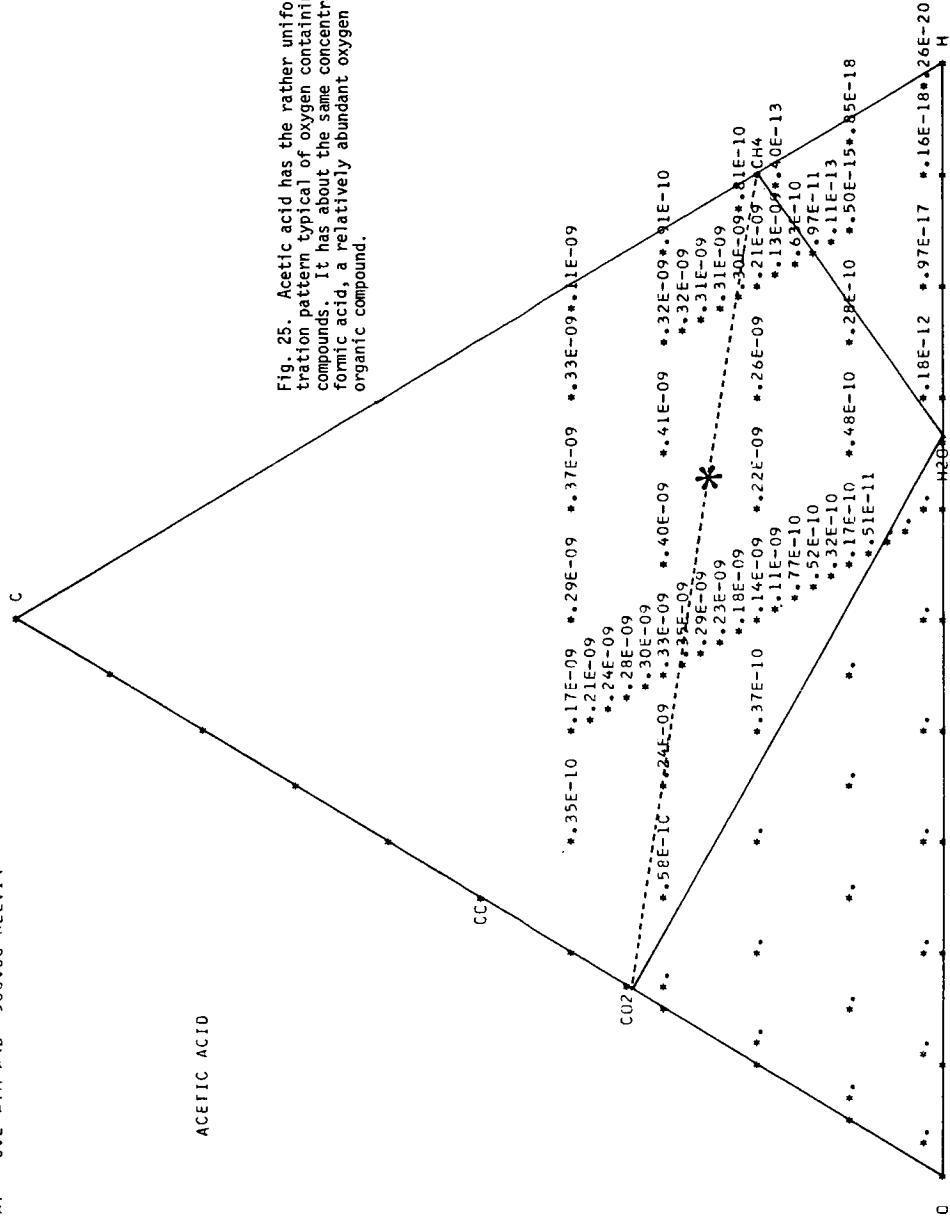


Fig. 25. Acetic acid has the rather uniform concentration pattern typical of oxygen containing organic compounds. It has about the same concentration as formic acid, a relatively abundant oxygen containing organic compound.

AT C.2 ATM AND 500.00 KELVIN

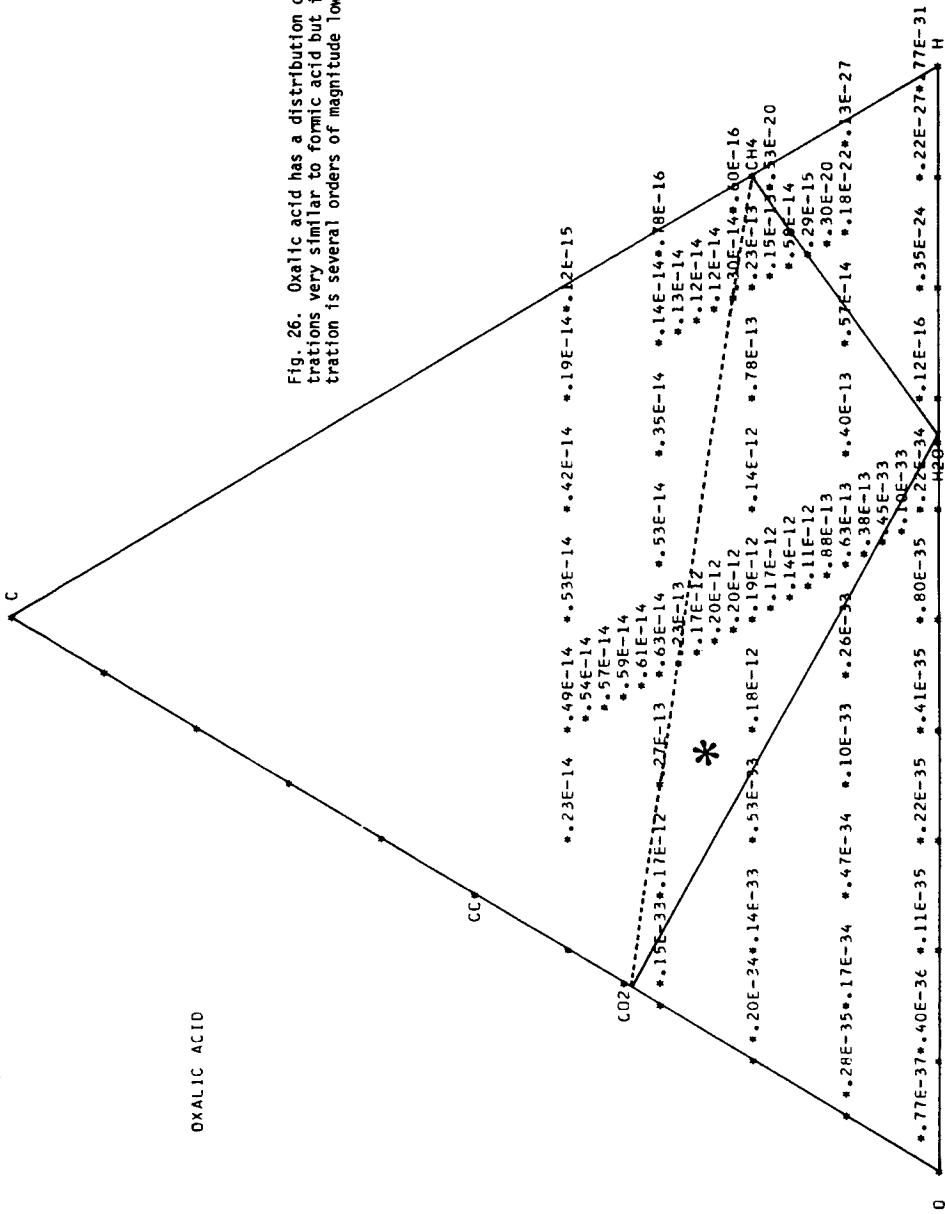


Fig. 26. Oxalic acid has a distribution of concentrations very similar to formic acid but its concentration is several orders of magnitude lower.

TABLE 2a

500°K AND 1 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{\partial F}{\partial n}$ /RT,  
FOR 68 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER OF  
MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-98.161	-28.692	-0.849	-0.109
2	2.0	9.0	89.0	-98.038	-27.908	-0.907	-0.105
3	2.0	19.0	79.0	-97.832	-27.480	-1.005	-0.100
4	2.0	29.0	69.0	-97.572	-27.201	-1.130	-0.095
5	2.0	39.0	59.0	-97.219	-26.962	-1.301	-0.090
6	2.0	49.0	49.0	-96.670	-26.708	-1.570	-0.084
7	2.0	59.0	39.0	-95.354	-26.284	-2.223	-0.079
8	2.0	69.0	29.0	-2.973	-2.431	-49.945	-0.076
9	2.0	79.0	19.0	-7.127	-1.385	-52.470	-0.085
10	2.0	89.0	9.0	-8.335	-1.085	-53.831	-0.094
11	2.0	96.0	2.0	-8.671	-0.954	-55.605	-0.100
12	10.0	2.0	88.0	-96.245	-28.612	-0.994	-0.100
13	10.0	10.0	80.0	-96.048	-27.756	-1.088	-0.096
14	10.0	20.0	70.0	-95.729	-27.327	-1.242	-0.091
15	10.0	30.0	60.0	-95.259	-27.004	-1.472	-0.086
16	10.0	40.0	50.0	-94.343	-26.629	-1.925	-0.081
17	10.0	50.0	40.0	-0.695	-3.130	-48.805	-0.076
18	10.0	60.0	30.0	-0.116	-2.911	-49.358	-0.071
19	10.0	70.0	20.0	-0.305	-2.720	-49.876	-0.066
20	10.0	80.0	10.0	-4.585	-1.610	-52.631	-0.069
21	10.0	88.0	2.0	-6.078	-1.240	-54.993	-0.077
22	20.0	2.0	78.0	-94.558	-28.458	-1.280	-0.090
23	20.0	10.0	70.0	-94.566	-27.553	-1.472	-0.086
24	20.0	20.0	60.0	-93.650	-26.975	-1.925	-0.081
25	20.0	30.0	50.0	0.789	-3.367	-48.920	-0.076
26	20.0	40.0	40.0	1.122	-3.216	-49.441	-0.070
27	20.0	50.0	30.0	1.559	-3.181	-49.797	-0.065
28	20.0	60.0	20.0	1.956	-3.187	-50.191	-0.059
29	20.0	70.0	10.0	2.471	-3.247	-50.784	-0.054
30	22.0	76.0	2.0	9.610	-4.665	-54.375	-0.203
31	18.0	80.0	2.0	-0.913	-2.373	-52.684	-0.052
32	30.0	2.0	68.0	-92.888	-28.037	-2.102	-0.080
33	30.0	10.0	60.0	2.137	-3.820	-49.632	-0.075
34	30.0	20.0	50.0	6.899	-4.657	-52.079	-0.070
35	30.0	30.0	40.0	9.911	-5.317	-53.694	-0.064
36	30.0	40.0	30.0	9.908	-5.248	-53.831	-0.058
37	30.0	50.0	20.0	9.896	-5.191	-54.023	-0.052
38	30.0	60.0	10.0	9.884	-5.142	-54.360	-0.046
39	30.0	68.0	2.0	9.874	-5.108	-55.166	-0.040
40	40.0	10.0	50.0	10.397	-6.069	-53.824	-0.062
41	40.0	20.0	40.0	10.163	-5.621	-53.812	-0.056
42	40.0	30.0	30.0	10.078	-5.452	-53.908	-0.050
43	40.0	40.0	20.0	10.026	-5.345	-54.080	-0.043
44	40.0	50.0	10.0	9.989	-5.265	-54.404	-0.037
45	40.0	58.0	2.0	9.965	-5.214	-55.204	-0.031
46	12.0	78.0	10.0	-3.077	-1.939	-51.962	-0.063
47	14.0	76.0	10.0	-0.254	-2.609	-50.677	-0.058
48	16.0	74.0	10.0	0.811	-2.859	-50.448	-0.056
49	18.0	72.0	10.0	1.549	-3.030	-50.513	-0.055
50	22.0	68.0	10.0	7.559	-4.506	-53.198	-0.052
51	24.0	66.0	10.0	9.782	-5.074	-54.313	-0.051
52	26.0	64.0	10.0	9.828	-5.099	-54.335	-0.049
53	28.0	62.0	10.0	9.859	-5.121	-54.349	-0.047
54	4.0	56.0	40.0	-94.343	-26.230	-2.381	-0.079
55	6.0	54.0	40.0	-92.550	-25.901	-3.074	-0.077
56	8.0	52.0	40.0	-1.397	-3.214	-48.532	-0.077
57	12.0	48.0	40.0	-0.257	-3.113	-48.956	-0.075
58	14.0	46.0	40.0	0.104	-3.119	-49.078	-0.074
59	16.0	44.0	40.0	0.438	-3.139	-49.191	-0.073
60	18.0	42.0	40.0	0.770	-3.171	-49.309	-0.071
61	22.0	38.0	40.0	1.524	-3.280	-49.602	-0.069
62	24.0	36.0	40.0	2.034	-3.375	-49.820	-0.068
63	26.0	34.0	40.0	2.828	-3.545	-50.181	-0.067
64	28.0	32.0	40.0	7.090	-4.584	-52.282	-0.066
65	32.0	28.0	40.0	9.970	-5.364	-53.722	-0.063
66	34.0	26.0	40.0	10.017	-5.413	-53.744	-0.061
67	36.0	24.0	40.0	10.061	-5.469	-53.764	-0.059
68	38.0	22.0	40.0	10.108	-5.536	-53.786	-0.058

TABLE 2b

500°K AND 1 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	4.9E-03	2.1E-02	3.1E-02	4.4E-02	7.3E-02	6.1E-02	0.
H2	1.9E-03	1.6E-03	2.4E-05	4.0E-02	1.5E-03	3.4E-05	1.8E-24
O2	0.	0.	0.	0.	0.	0.	8.3E-02
WATER	9.6E-02	4.3E-02	9.1E-06	4.4E-02	1.0E-02	6.6E-06	4.2E-02
CO	5.8E-06	1.9E-05	1.7E-03	2.6E-09	1.9E-05	8.7E-04	1.4E-26
CO2	3.8E-02	6.6E-02	8.7E-02	3.7E-07	1.7E-02	2.2E-02	4.2E-02
BENZENE	7.5E-28	2.4E-23	6.5E-06	5.0E-34	6.6E-20	1.6E-05	0.
NAPHTHALENE	0.	4.5E-37	3.3E-06	0.	2.5E-31	1.0E-05	0.
ASPHALT	0.	0.	5.3E-04	0.	0.	2.4E-03	0.
N2	8.6E-01	8.7E-01	8.8E-01	8.7E-01	9.0E-01	9.1E-01	8.3E-01
NH3	2.5E-05	2.0E-05	3.6E-08	2.4E-03	1.8E-05	6.2E-08	7.4E-37
HYDRAZINE	1.5E-27	1.1E-27	2.5E-31	6.7E-25	9.9E-28	5.1E-31	0.
NO	9.6E-31	5.1E-31	7.3E-33	2.1E-32	1.4E-31	3.8E-33	4.3E-10
NO2	0.	0.	0.	0.	0.	0.	1.4E-08
N2O	1.9E-34	1.0E-34	1.4E-36	4.1E-36	2.7E-35	7.7E-37	8.2E-14
N03	0.	0.	0.	0.	0.	0.	9.8E-18
N2O3	0.	0.	0.	0.	0.	0.	5.1E-21
N2O4	0.	0.	0.	0.	0.	0.	1.5E-19
N2O5	0.	0.	0.	0.	0.	0.	2.3E-23
NITROUS ACID	0.	0.	0.	0.	0.	0.	1.2E-11
NITRIC ACID	0.	0.	0.	0.	0.	0.	7.2E-11
NH2CH	8.5E-18	3.5E-18	9.1E-23	1.8E-17	8.4E-19	8.1E-23	1.1E-28
NITROMETHANE	0.	0.	0.	0.	0.	0.	0.
HCN	3.0E-14	1.7E-13	1.4E-10	2.9E-15	6.5E-13	1.6E-10	0.
C2N2	1.3E-31	4.8E-30	2.1E-22	5.4E-35	7.4E-29	2.1E-22	0.
CYANAMIDE	8.0E-23	4.2E-22	4.1E-20	3.4E-23	1.6E-21	5.9E-20	0.
HNCC	4.4E-13	1.3E-12	1.5E-11	9.0E-16	1.3E-12	9.2E-12	0.
METHYL CYANIDE	2.0E-17	5.9E-16	4.7E-11	8.0E-19	8.1E-15	7.6E-11	0.
ME1H-ISCCYANIDE	7.3E-24	2.1E-22	1.7E-17	2.9E-25	3.0E-21	2.8E-17	0.
ETHYL CYCRAZINE	3.5E-35	6.8E-34	1.5E-33	2.8E-33	8.1E-33	5.9E-33	0.
ETHYLENEIMINE	7.7E-25	1.9E-23	2.3E-20	6.5E-25	2.5E-22	5.3E-20	0.
METHYL AMINE	4.1E-15	1.7E-14	3.0E-15	1.7E-13	5.6E-14	7.1E-15	0.
DIMETHYL AMINE	1.1E-23	2.4E-22	4.2E-21	2.0E-22	2.9E-21	1.4E-20	0.
TRIMETHYL AMINE	4.2E-31	4.5E-29	7.9E-26	3.1E-30	2.0E-27	3.6E-25	0.
ETHENYL AMINE	1.7E-30	4.2E-29	5.0E-26	1.4E-30	5.4E-28	1.1E-25	0.
DIAMINOCETHANE	1.0E-32	1.9E-31	4.3E-31	8.1E-31	2.3E-30	1.7E-30	0.
IMICAZOLE	3.8E-35	6.3E-33	4.0E-25	1.4E-37	3.3E-31	7.7E-25	0.
SYMMET. TRIAZINE	1.0E-36	1.8E-34	9.7E-26	0.	1.0E-32	1.6E-25	0.
NH2SYM. TRIAZINE	0.	0.	2.0E-36	0.	0.	4.0E-36	0.
ANILINE	1.9E-37	5.8E-33	1.9E-16	0.	1.6E-29	5.6E-16	0.
BENZONITRILE	0.	2.1E-34	3.0E-12	0.	2.3E-30	6.1E-12	0.
PHEN. ISCCYANIDE	0.	0.	1.1E-18	0.	8.3E-37	2.2E-18	0.
QUINOLINE	0.	0.	2.5E-12	0.	4.2E-35	6.9E-12	0.
PYRROLE	1.9E-32	1.8E-29	9.2E-19	6.7E-36	3.4E-27	2.0E-18	0.
PYRIDINE	9.3E-33	5.4E-29	1.8E-14	6.7E-38	4.0E-26	3.8E-14	0.
PYRIMIDINE	3.1E-33	3.2E-30	1.3E-18	2.4E-37	6.4E-28	2.5E-18	0.
PURINE	0.	0.	2.4E-39	0.	0.	4.6E-39	0.
ADENINE	0.	0.	0.	0.	0.	0.	0.
NICOTINIC ACID	1.5E-37	1.5E-33	6.6E-19	0.	2.9E-31	3.6E-19	0.
NICOTINAMIDE	0.	0.	1.6E-31	0.	0.	2.0E-31	0.
UREA	5.0E-32	1.2E-31	2.5E-33	9.8E-33	1.1E-31	2.6E-33	0.
FORMAMIDE	1.6E-22	4.1E-22	7.0E-23	6.9E-24	3.8E-22	6.1E-23	0.
ACETAMIDE	2.7E-26	3.6E-25	6.0E-24	5.0E-28	1.2E-24	7.2E-24	0.
METHOXYAMINE	6.5E-24	1.4E-23	3.6E-26	5.8E-24	1.2E-23	4.4E-26	0.
ETHANCLAMINE	5.2E-30	5.7E-29	1.5E-29	2.0E-30	1.8E-28	2.4E-29	0.
Α-ETHYLCHLAMINE	1.2E-33	1.3E-32	3.3E-33	4.5E-34	4.1E-32	5.5E-33	0.
Β-ETHYLCHLAMINE	1.9E-32	2.0E-31	5.2E-32	7.1E-33	6.5E-31	8.7E-32	0.
UXAMIC ACID	3.9E-29	1.7E-28	3.9E-29	1.6E-35	4.2E-29	8.7E-30	0.
CYANURIC ACID	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	2.2E-38	4.9E-37	0.	1.9E-38	1.5E-37	0.
ACETYLGLYCINE	0.	0.	2.2E-38	0.	0.	9.4E-39	0.
GLYCINE	5.0E-24	3.5E-23	8.4E-24	2.0E-27	3.1E-23	5.1E-24	0.
ALANINE	4.0E-30	1.4E-28	3.4E-27	6.7E-34	4.5E-28	2.8E-27	0.
PROLINE	0.	0.	2.0E-34	0.	0.	2.2E-34	0.
SERINE	6.4E-39	1.2E-37	4.1E-38	0.	1.0E-37	1.8E-38	0.
ASPARTIC ACID	4.9E-39	3.0E-37	9.4E-36	0.	2.5E-37	2.0E-36	0.
VALINE	0.	2.3E-39	5.3E-34	0.	9.8E-38	8.6E-34	0.
LEUCINE	0.	0.	2.1E-37	0.	0.	4.7E-37	0.
PHENYLALANINE	0.	0.	1.7E-31	0.	0.	2.5E-31	0.

AT 1.0 AM ANC 500 CC KELVIN

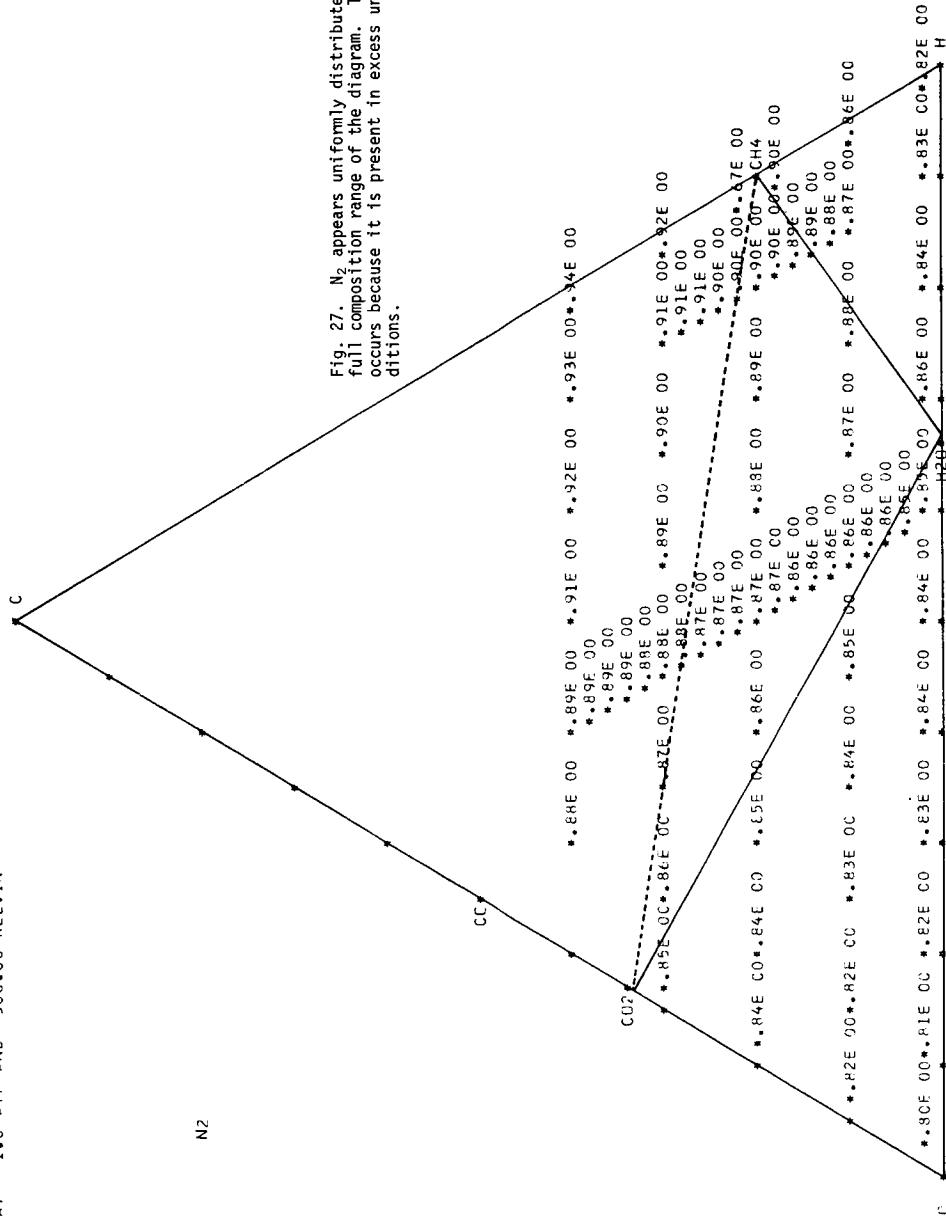


Fig. 27.  $N_2$  appears uniformly distributed over the full composition range of the diagram. This necessarily occurs because it is present in excess under these conditions.

AT 1.C AND 500.00 KELVIN

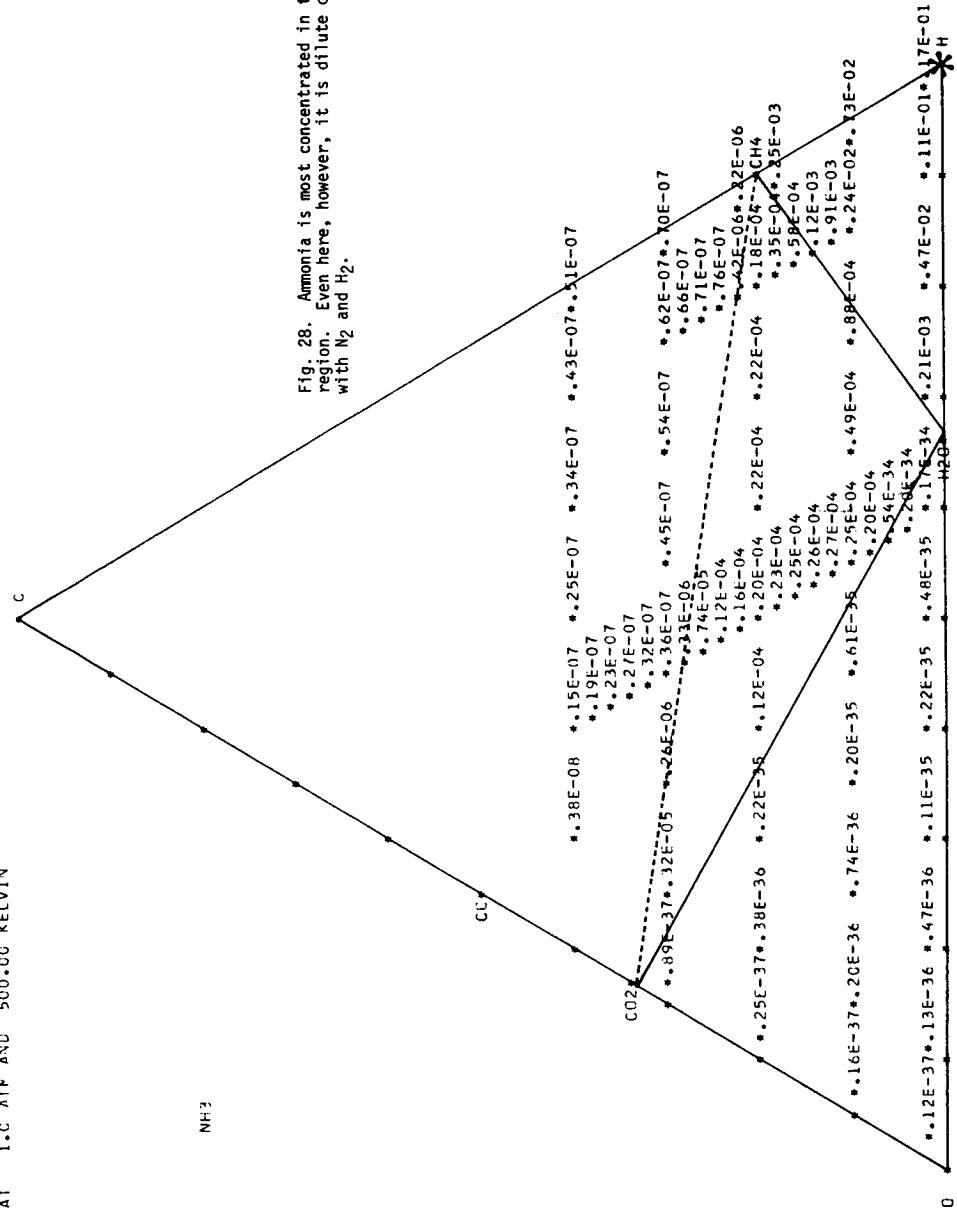
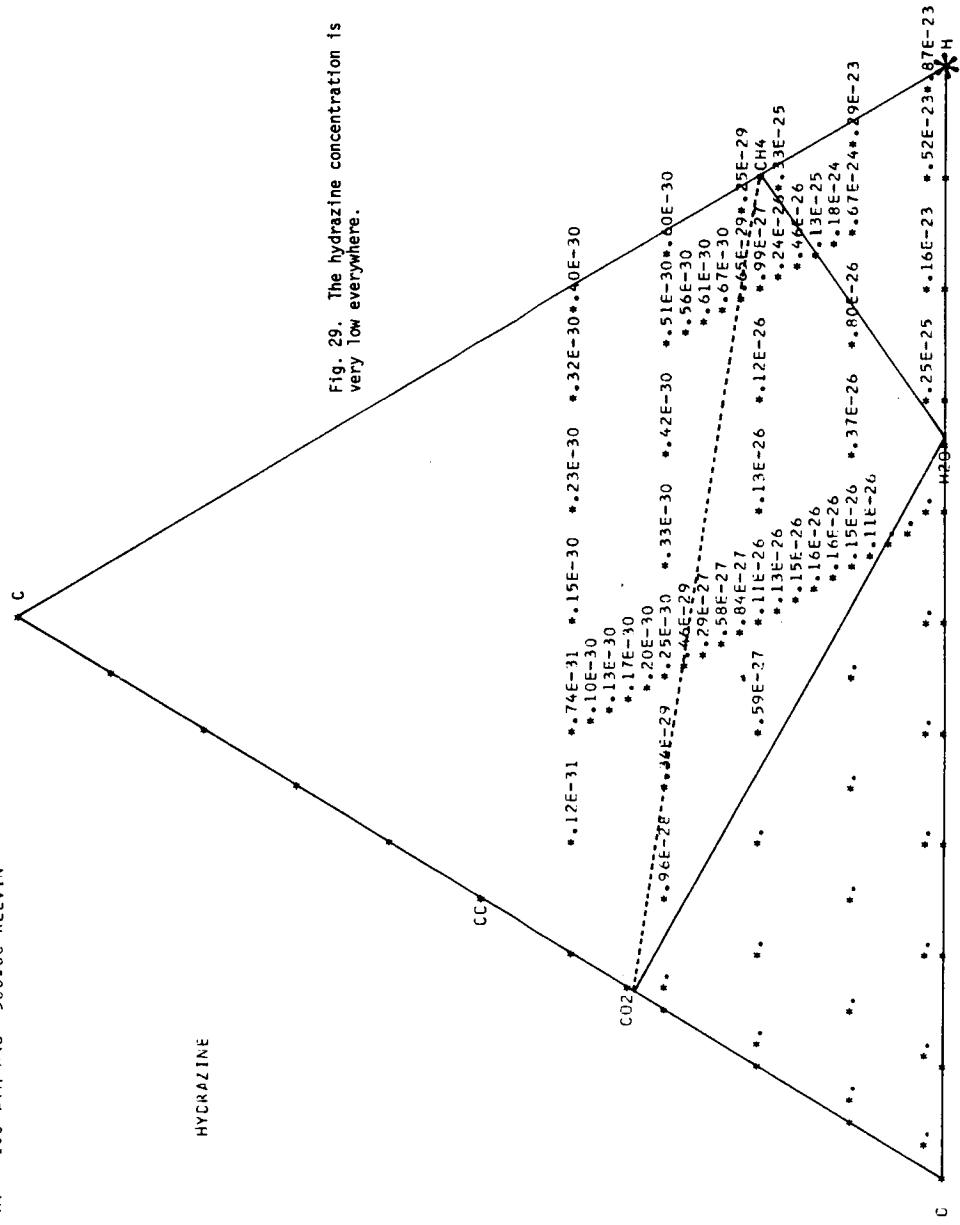
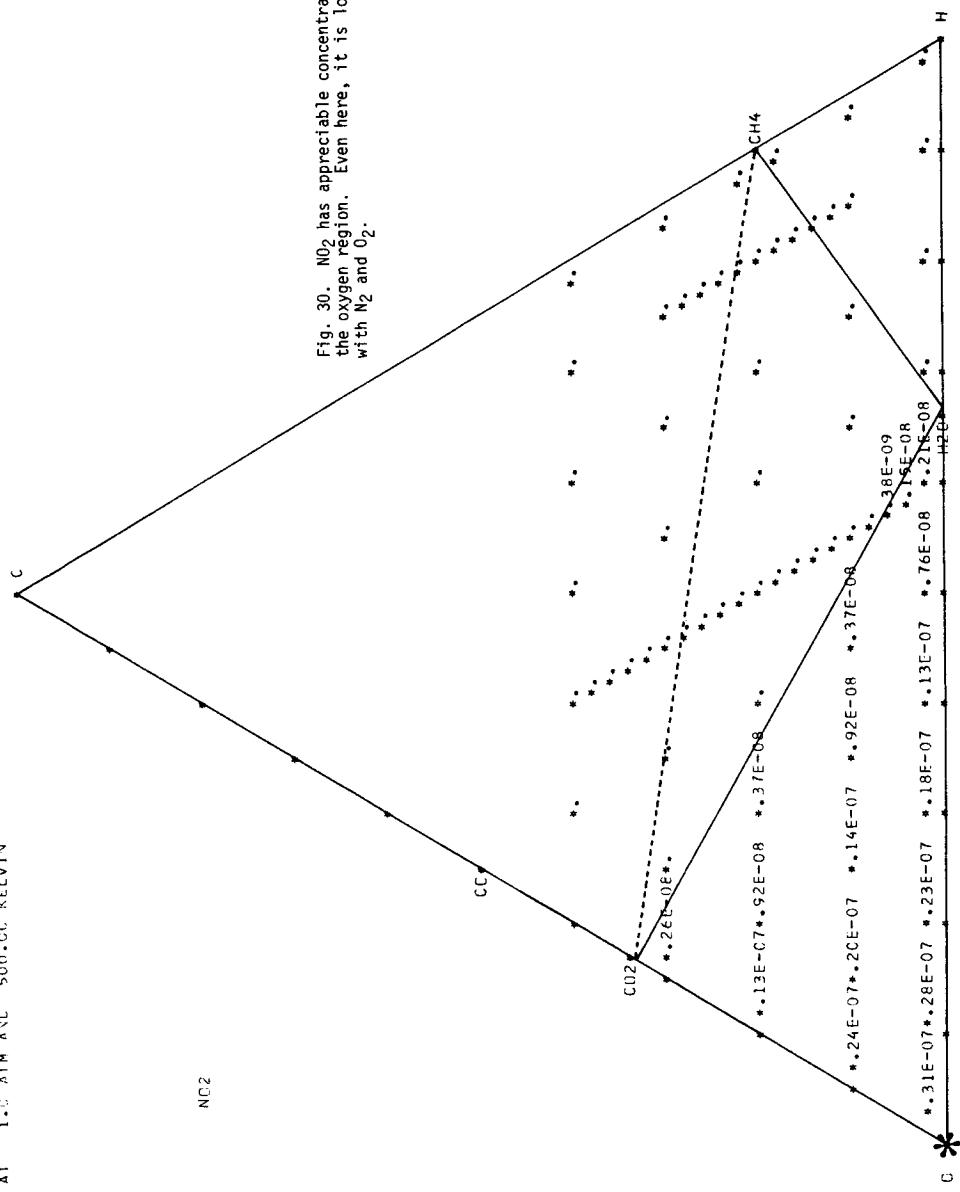


Fig. 28. Ammonia is most concentrated in the hydrogen region. Even here, however, it is dilute compared with  $\text{N}_2$  and  $\text{H}_2$ .

AT 1.0 ATM AND 500.00 KELVIN



AT 1.0 ATM AND 500.0°C KELVIN



$\Delta T$  1.C ATM AND 500.GC KELVIN

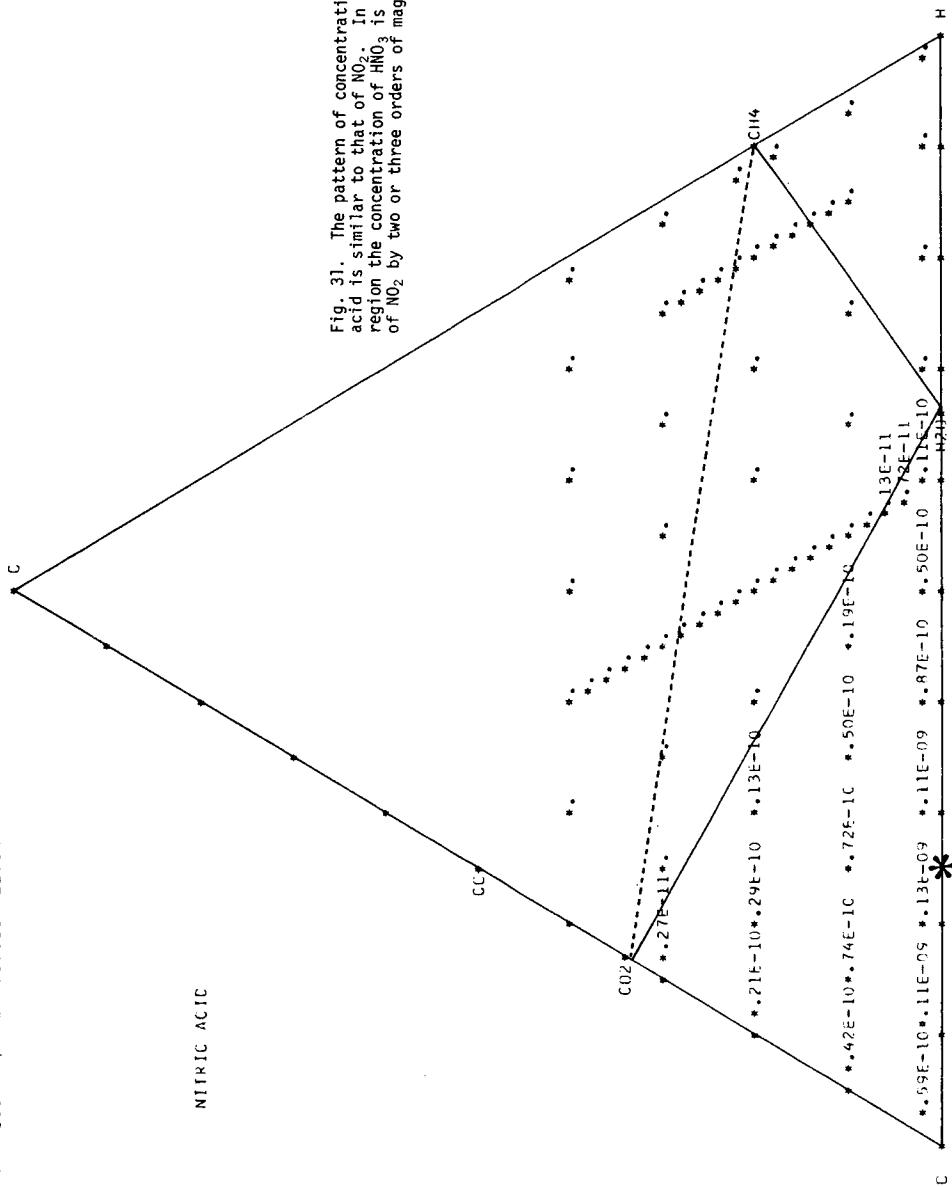


Fig. 31. The pattern of concentrations of nitric acid is similar to that of NO<sub>2</sub>. In the oxygen region the concentration of HNO<sub>3</sub> is less than that of NO<sub>2</sub> by two or three orders of magnitude.

AT 1.C ATM AND 500.0C KELVIN

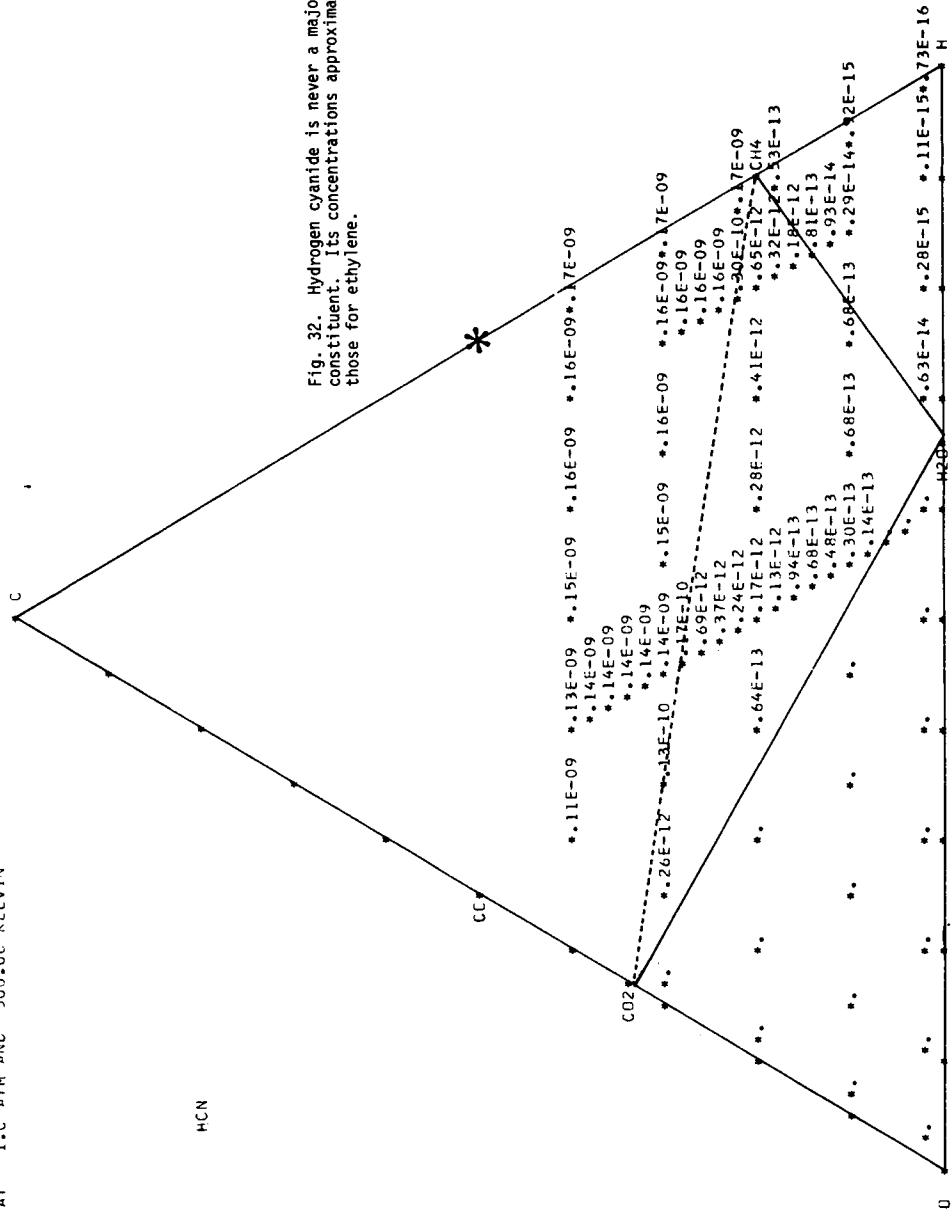


Fig. 32. Hydrogen cyanide is never a major constituent. Its concentrations approximate those for ethylene.

AT 1.0 ATM AND 500.00 KELVIN

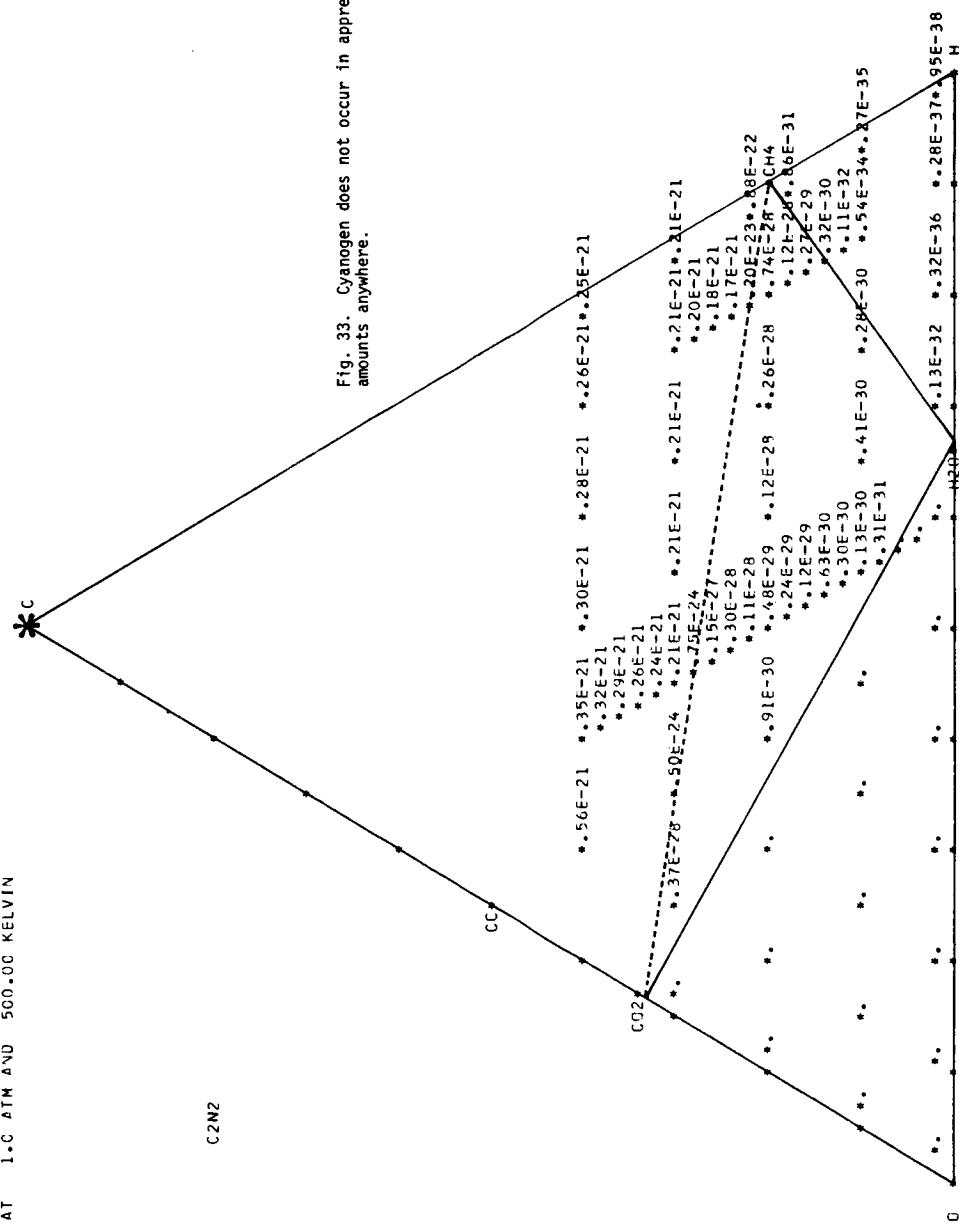


Fig. 33. Cyanogen does not occur in appreciable amounts anywhere.

AT 1.C ATM AND: 5CO+CC KELVIN

CYANAMIDE

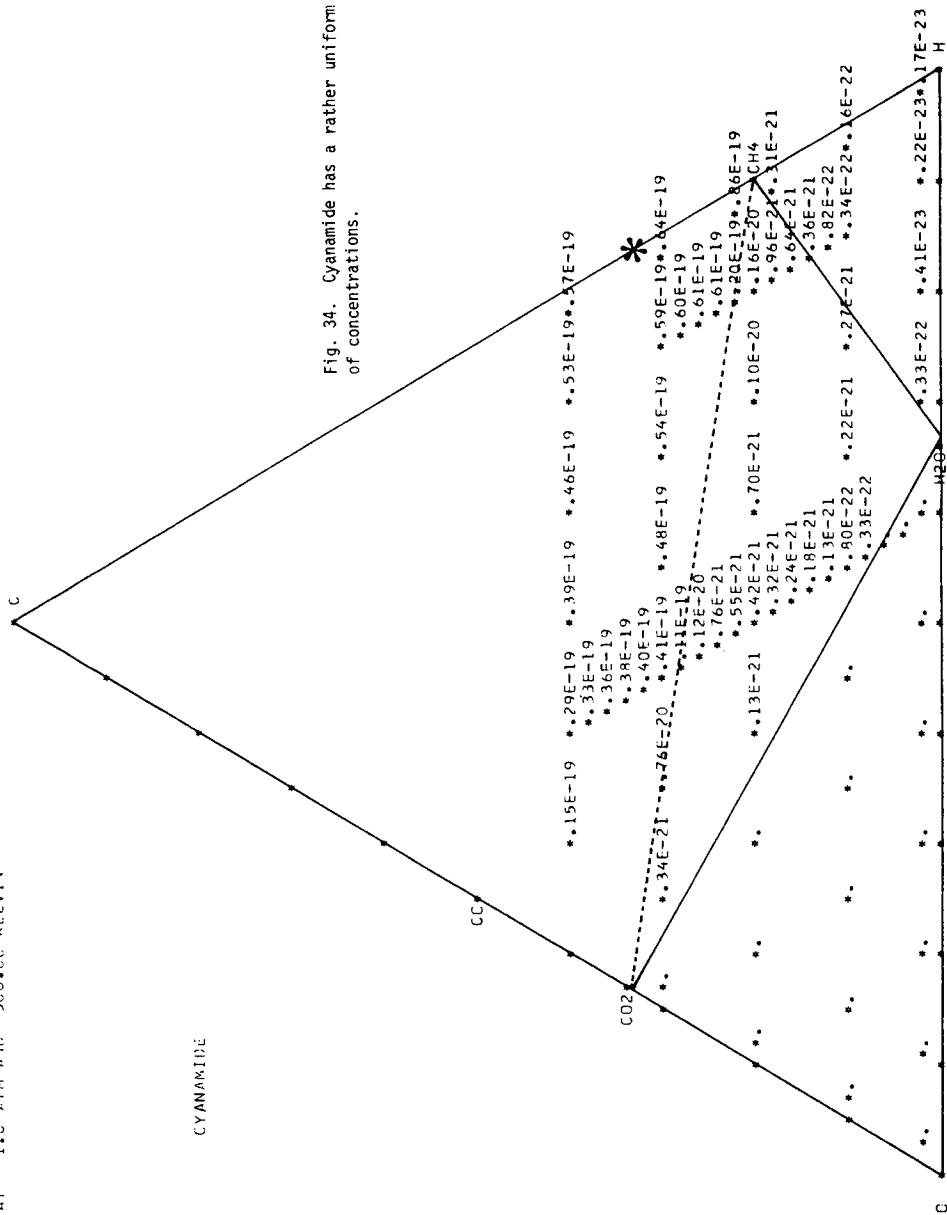


Fig. 34. Cyanamide has a rather uniform distribution of concentrations.

AT 1.0 ATM AND 500.00 KELVIN

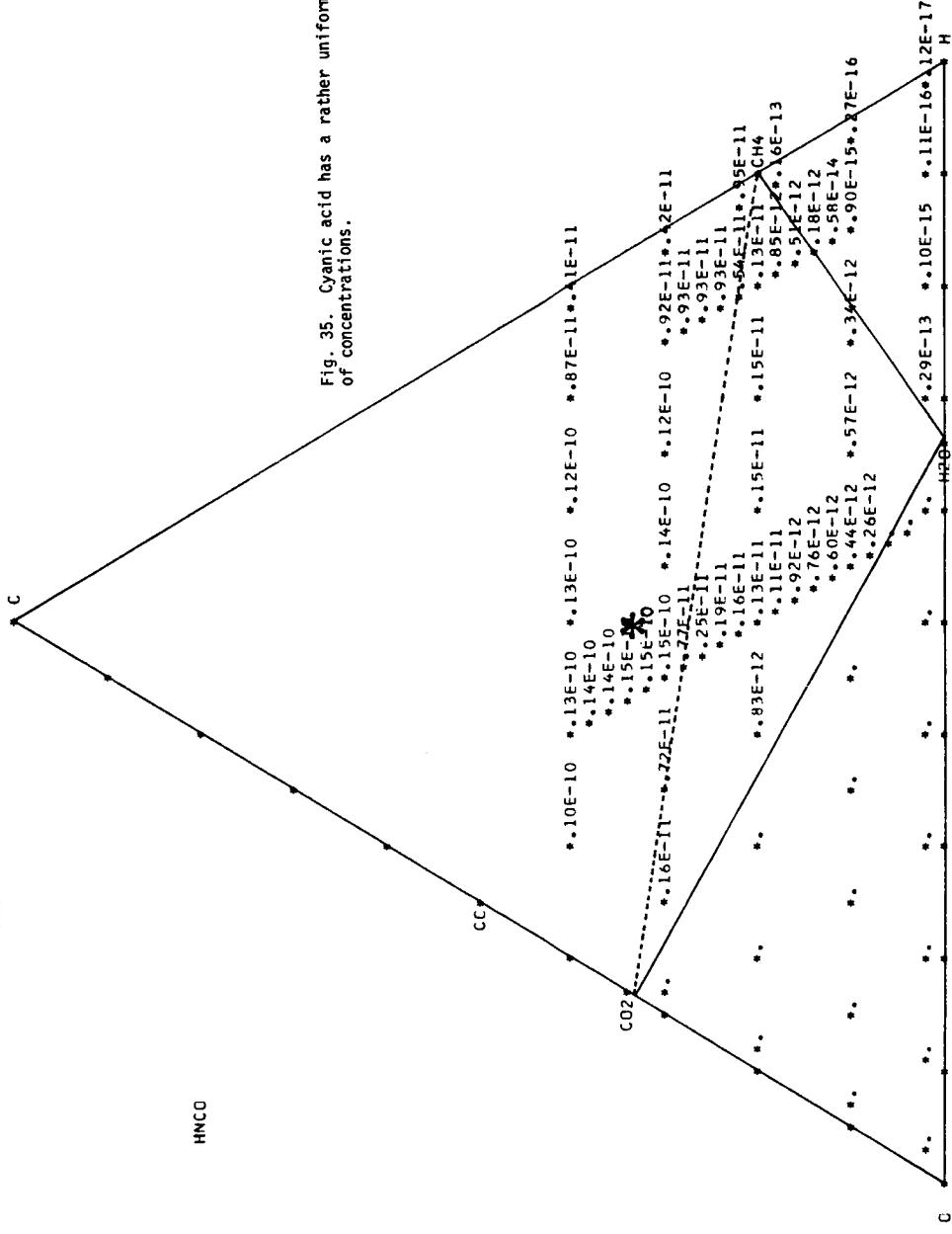
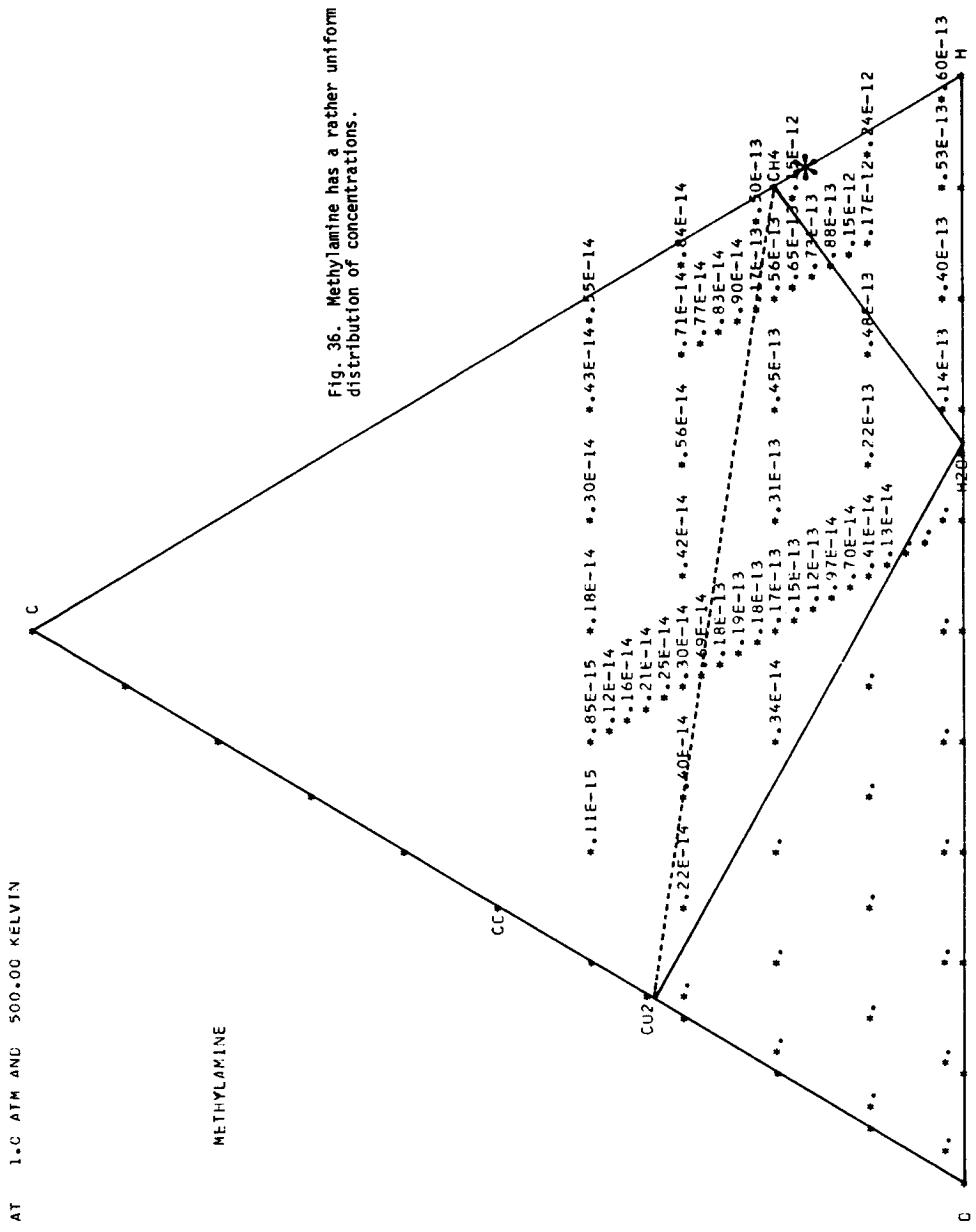
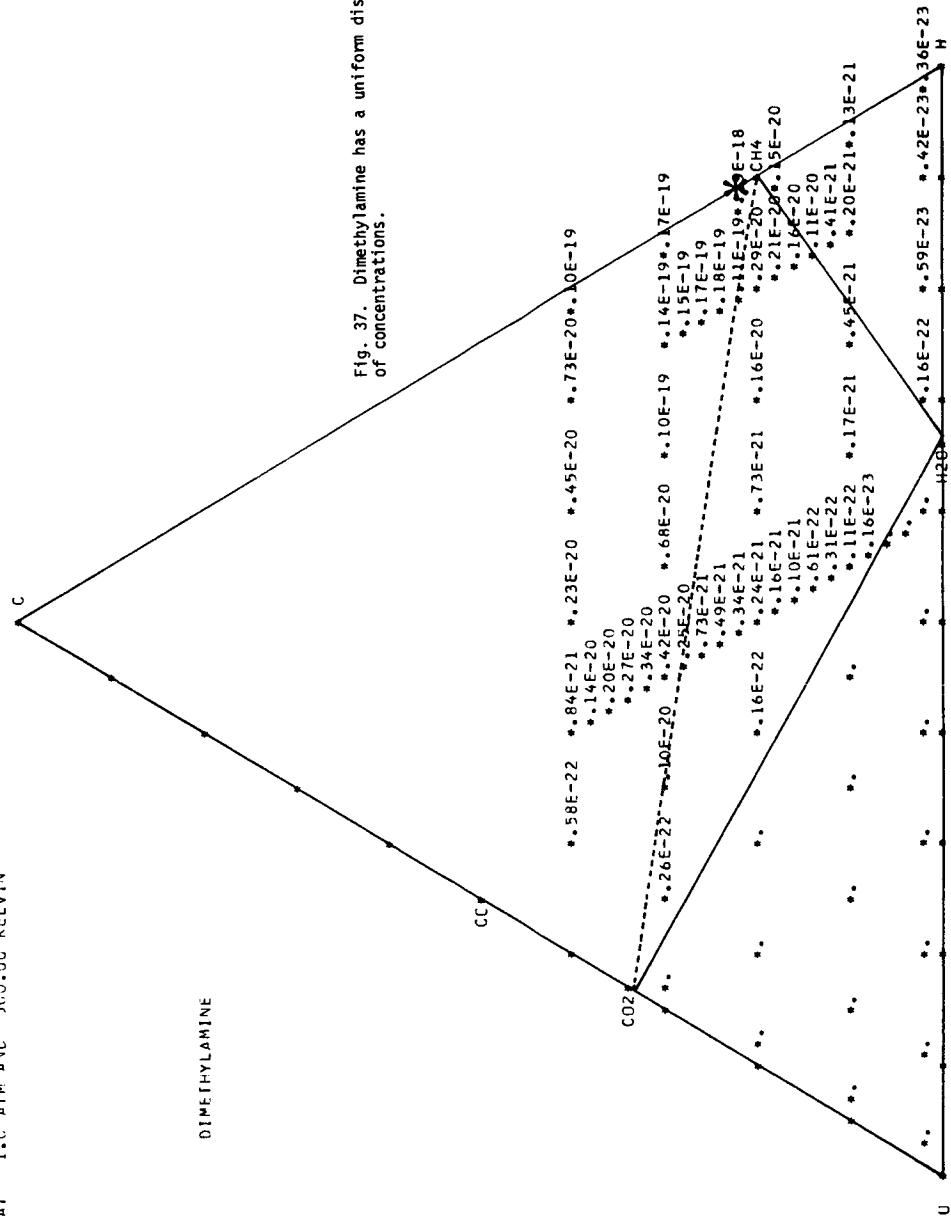


Fig. 35. Cyanic acid has a rather uniform distribution of concentrations.





AT 1.0 ATM AND 500.0°C KELVIN

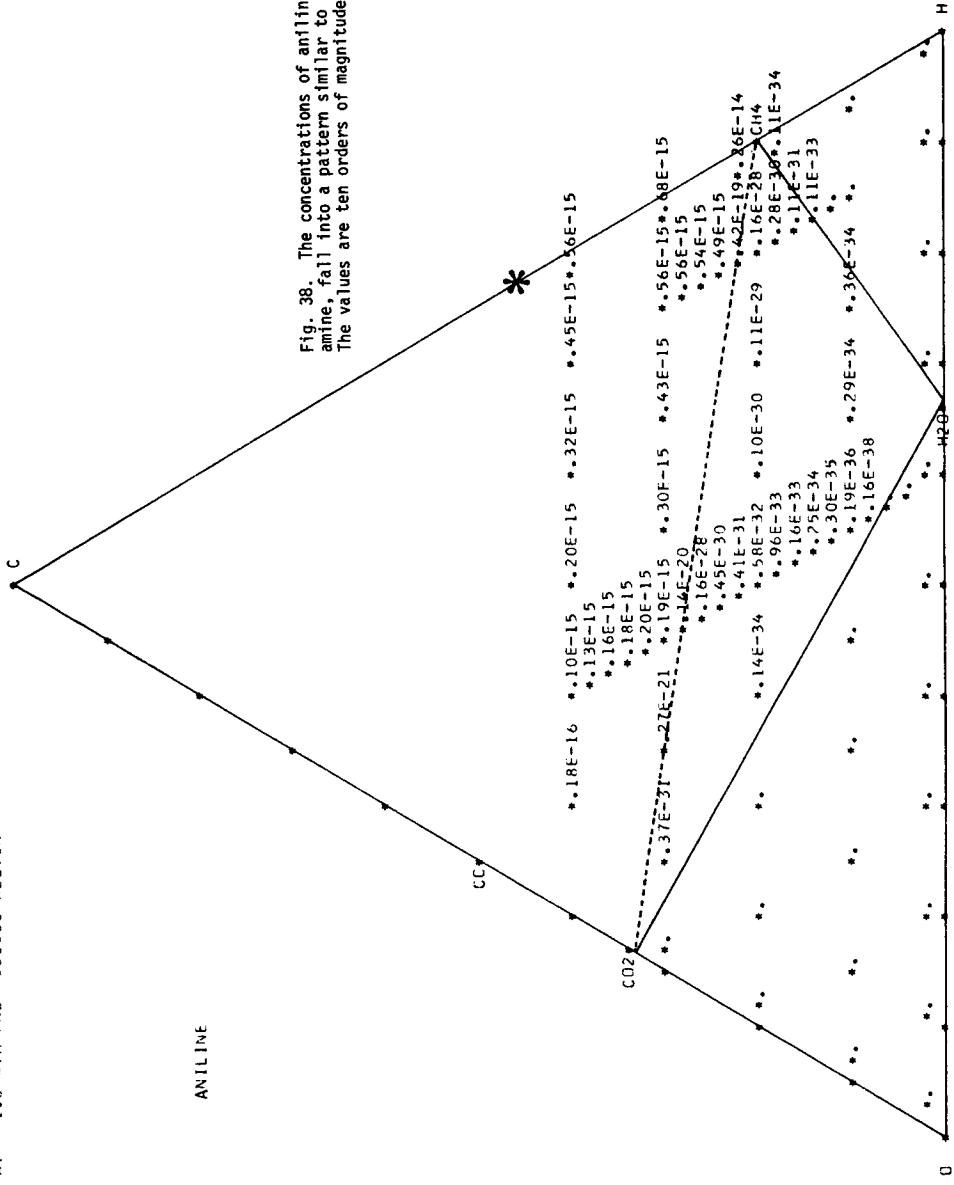


Fig. 38. The concentrations of aniline, an aromatic amine, fall into a pattern similar to that of benzene. The values are ten orders of magnitude lower.

AT 1.0 ATM ANC 500.00 KELVIN

PYRROLE

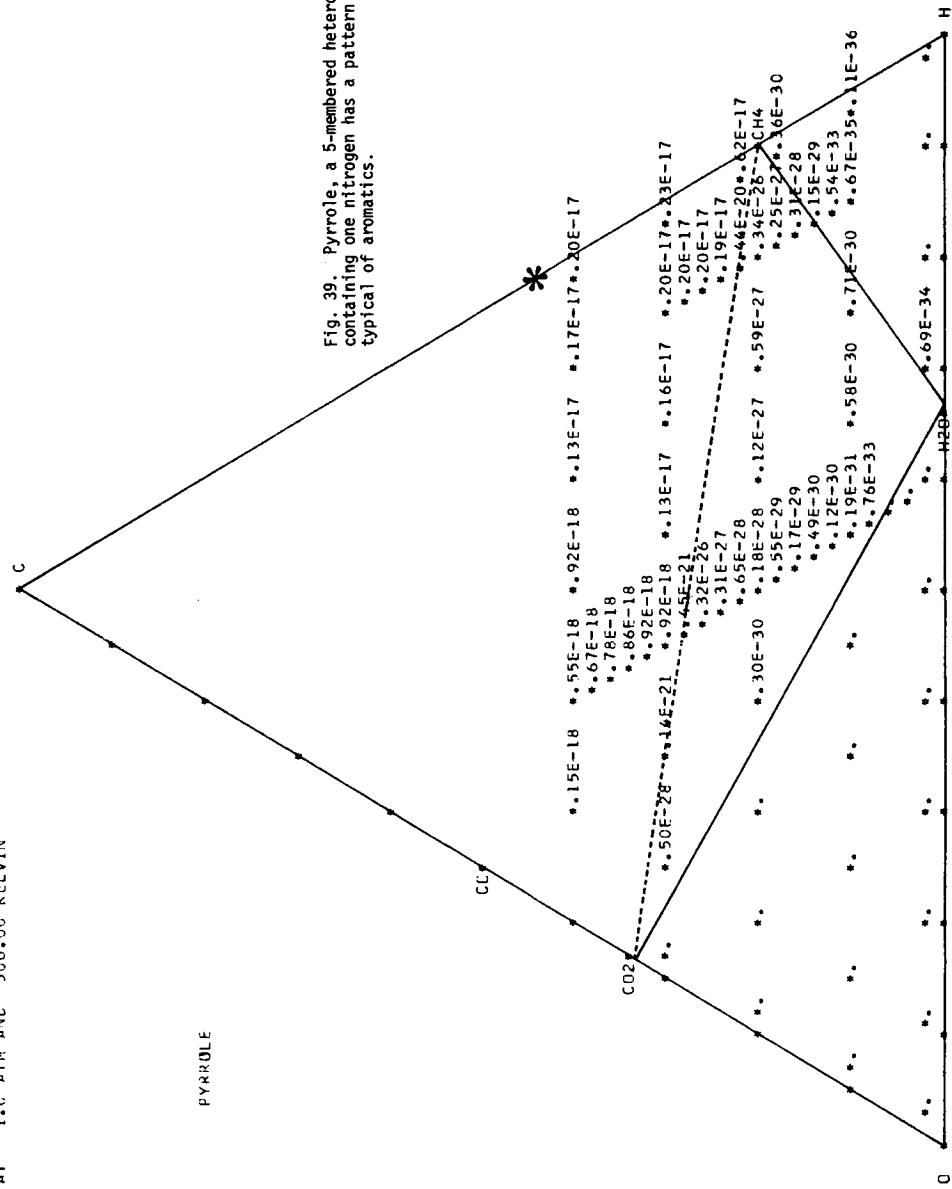


Fig. 39. Pyrrole, a 5-membered heterocyclic compound containing one nitrogen has a pattern of concentrations typical of aromatics.

AT 1.0 ATM AND 500.00 KELVIN

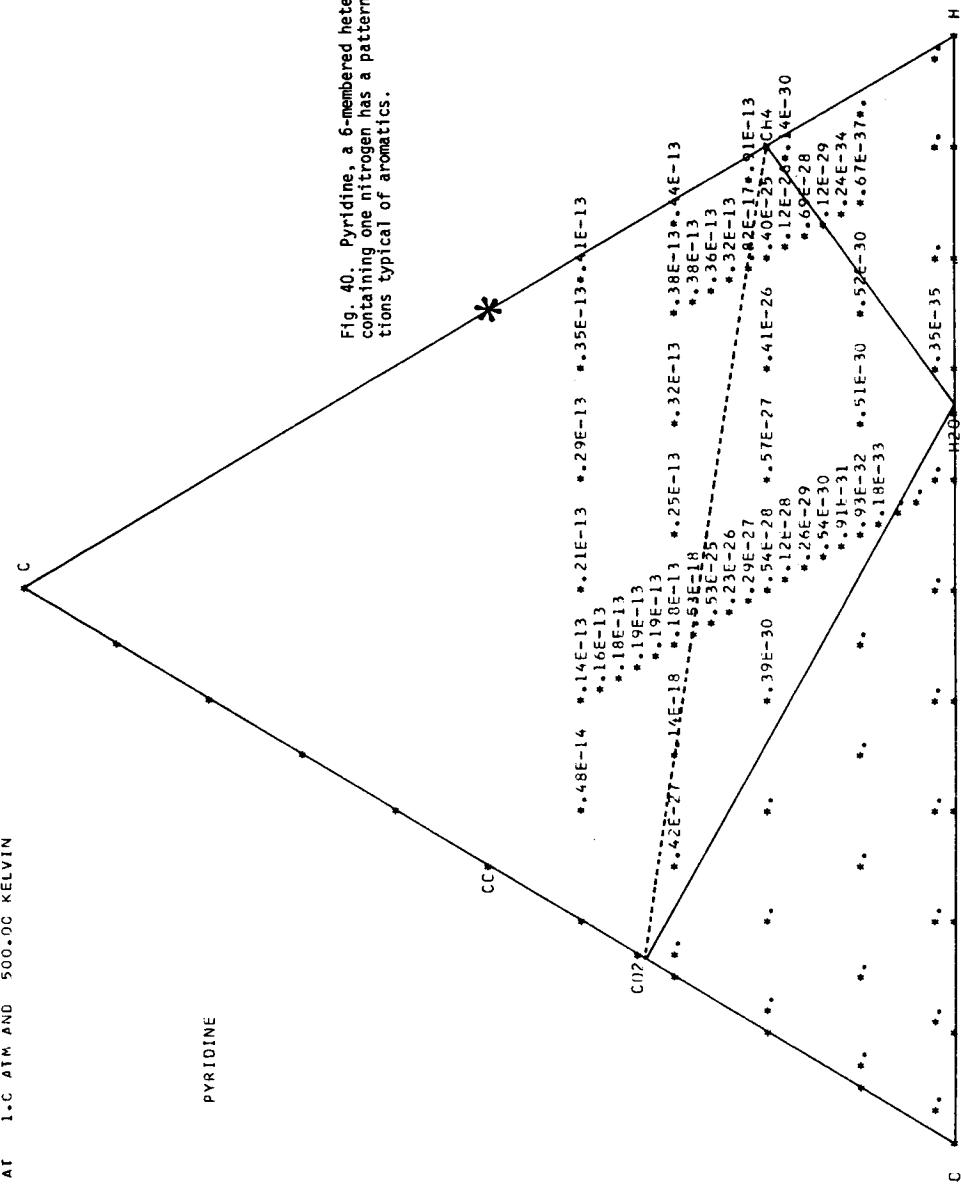


Fig. 40. Pyridine, a 6-membered heterocyclic compound containing one nitrogen has a pattern of concentrations typical of aromatics.

ATM 1.C ATM AND 100.CC KELVIN

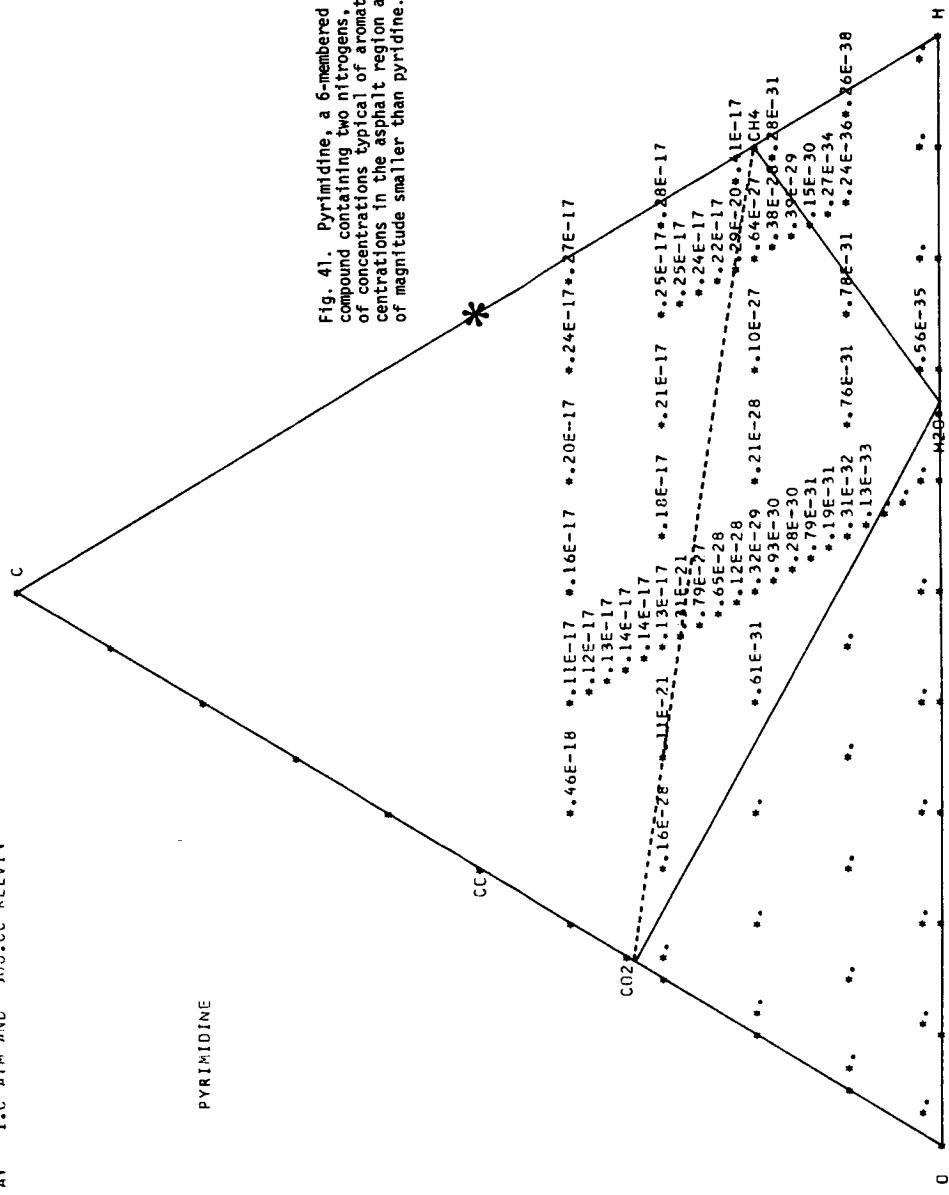


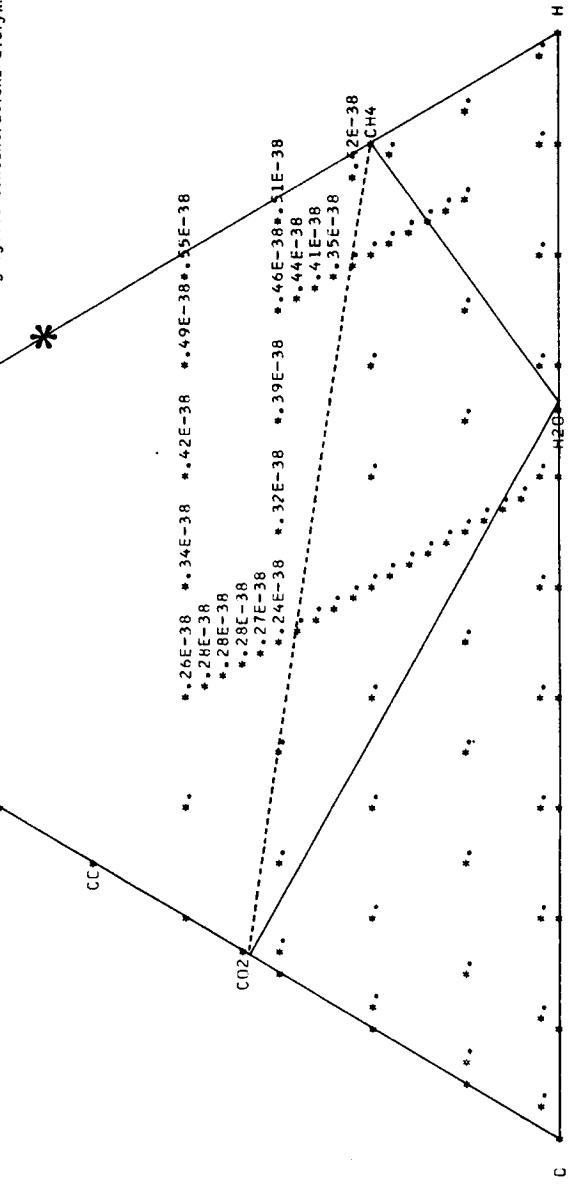
Fig. 41. Purimidine, a 6-membered heterocyclic compound containing two nitrogens, has a pattern of concentrations typical of aromatics. Its concentrations in the asphalt region are four orders of magnitude smaller than pyridine.

AT 1.0 ATM AND 500.00 KELVIN

PURINE

C

Fig. 42. Purine, the unsubstituted nucleus of the biologically important compounds adenine and guanine, has negligible concentrations everywhere.



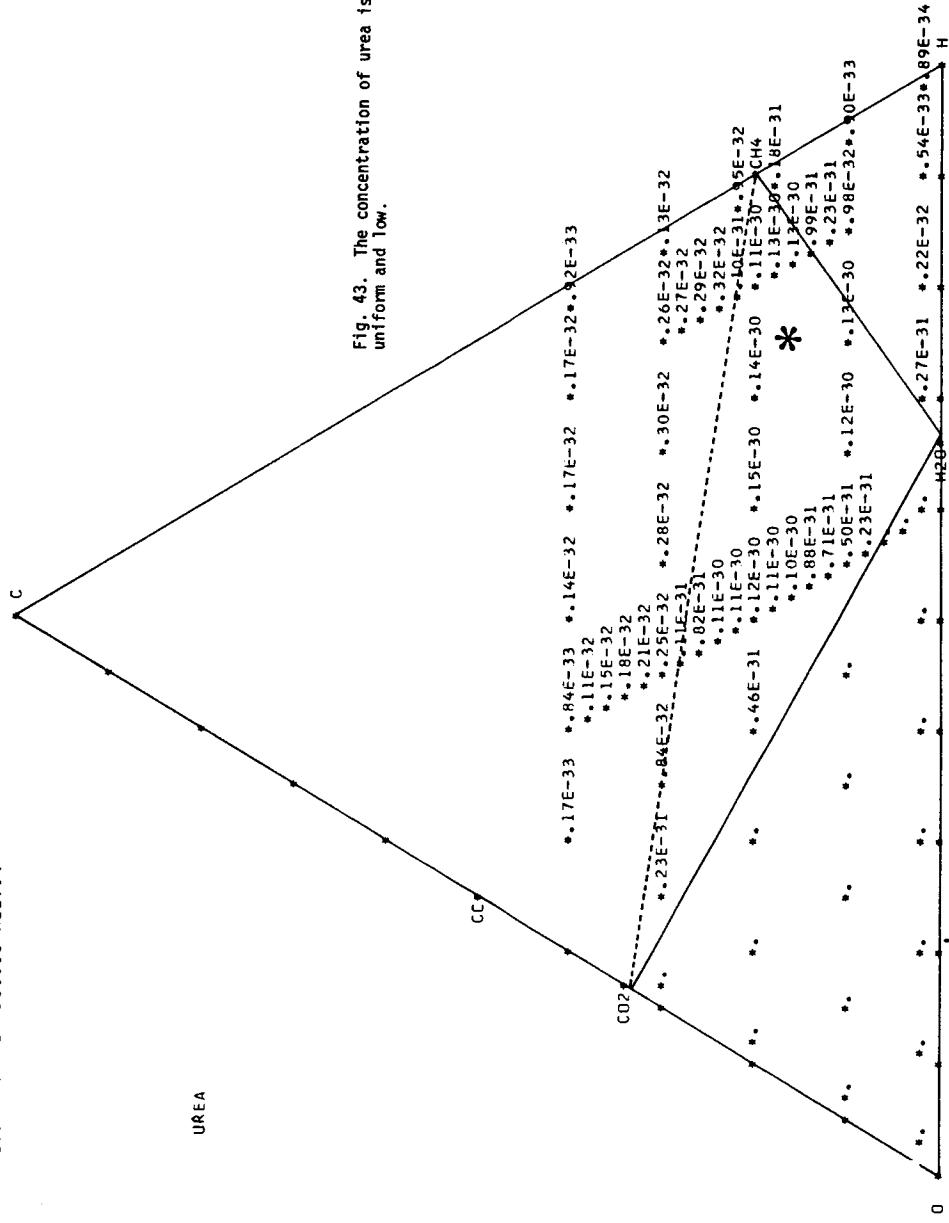
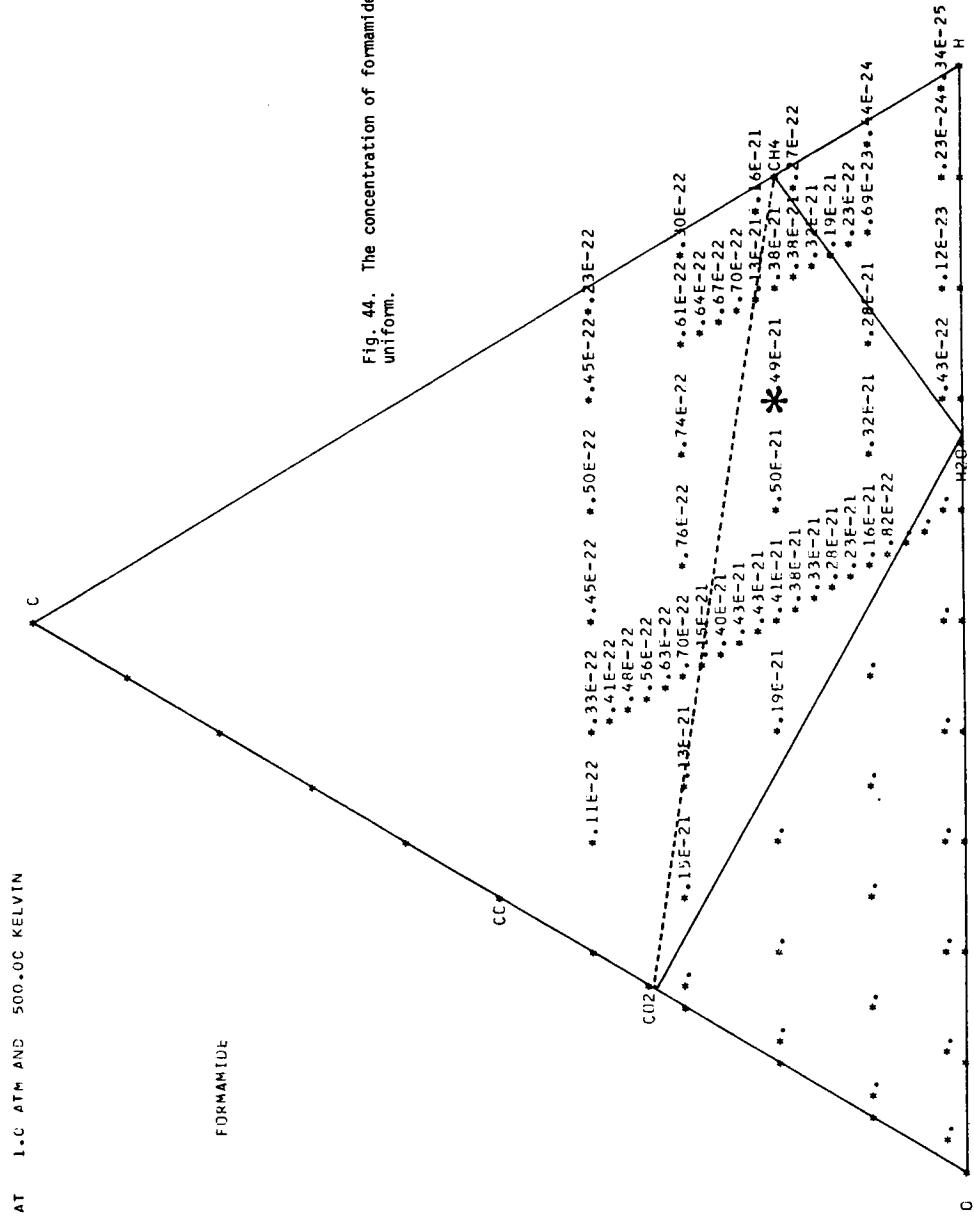


Fig. 43. The concentration of urea is rather uniform and low.

Fig. 44. The concentration of formamide is rather uniform.



ATM 1.0 ATM AND 500.0°C KELVIN

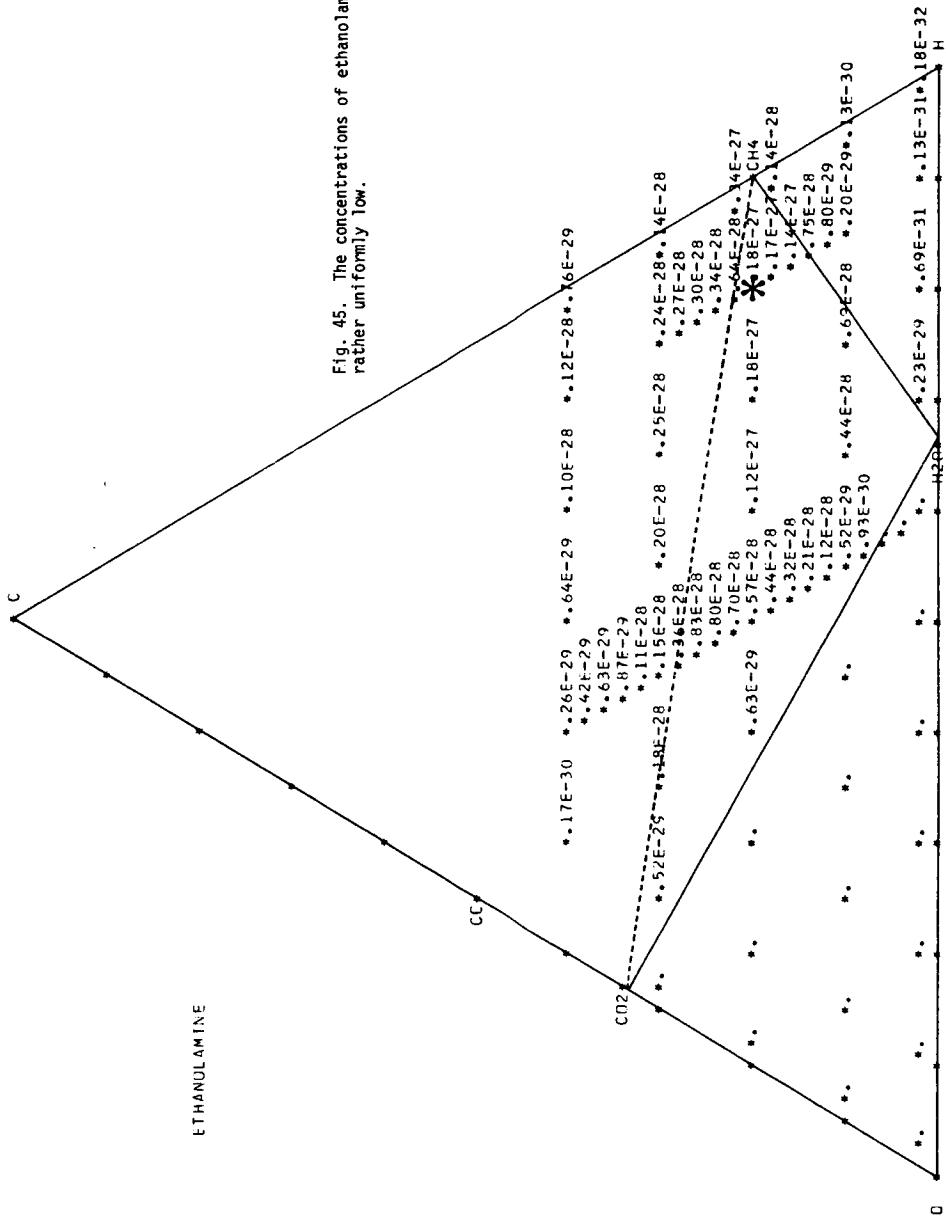


Fig. 45. The concentrations of ethanolamine are rather uniformly low.

AT 1.C ATM AND 500.CC KELVIN

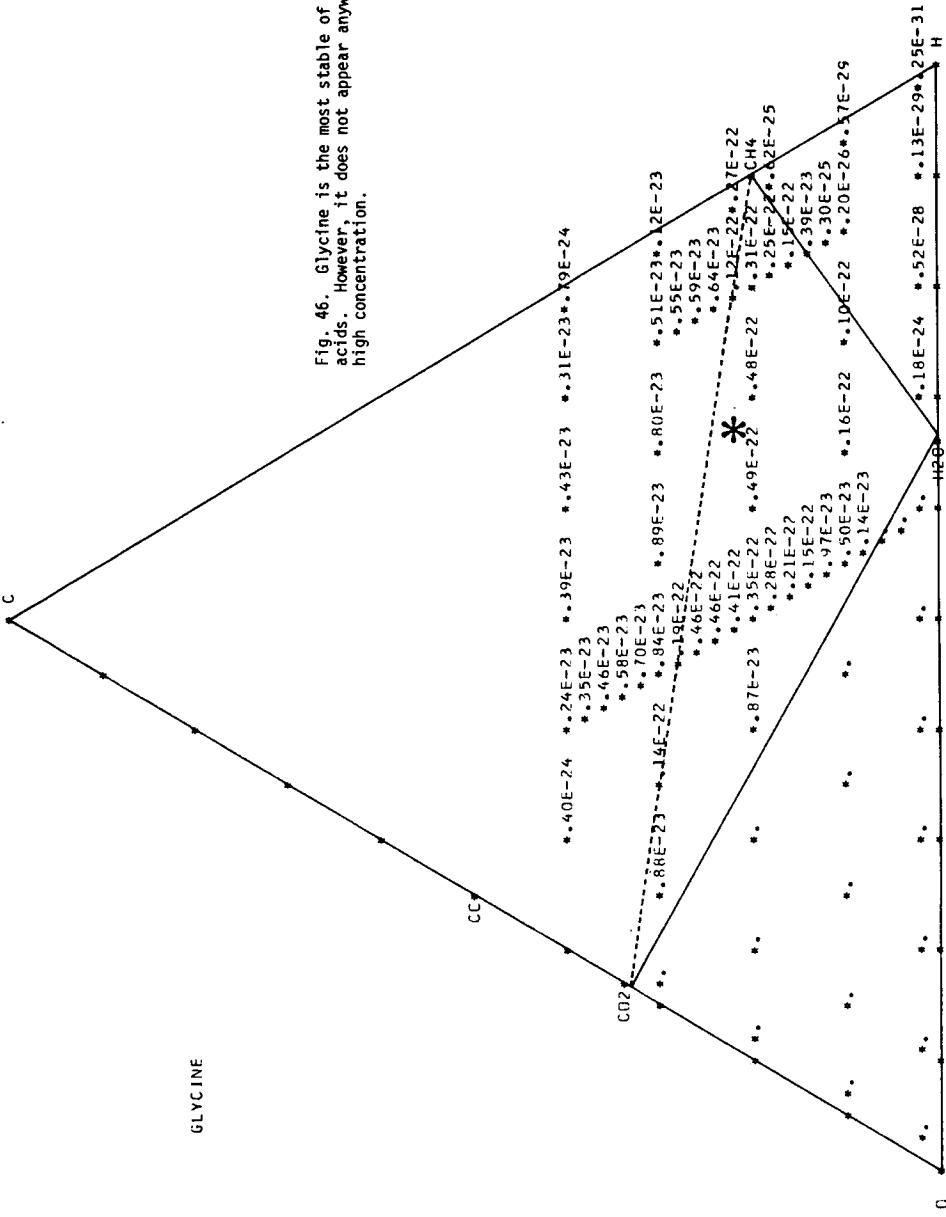


Fig. 46. Glycine is the most stable of the amino acids. However, it does not appear anywhere at high concentration.

AT 1.0 ATM AND 500.00 KELVIN

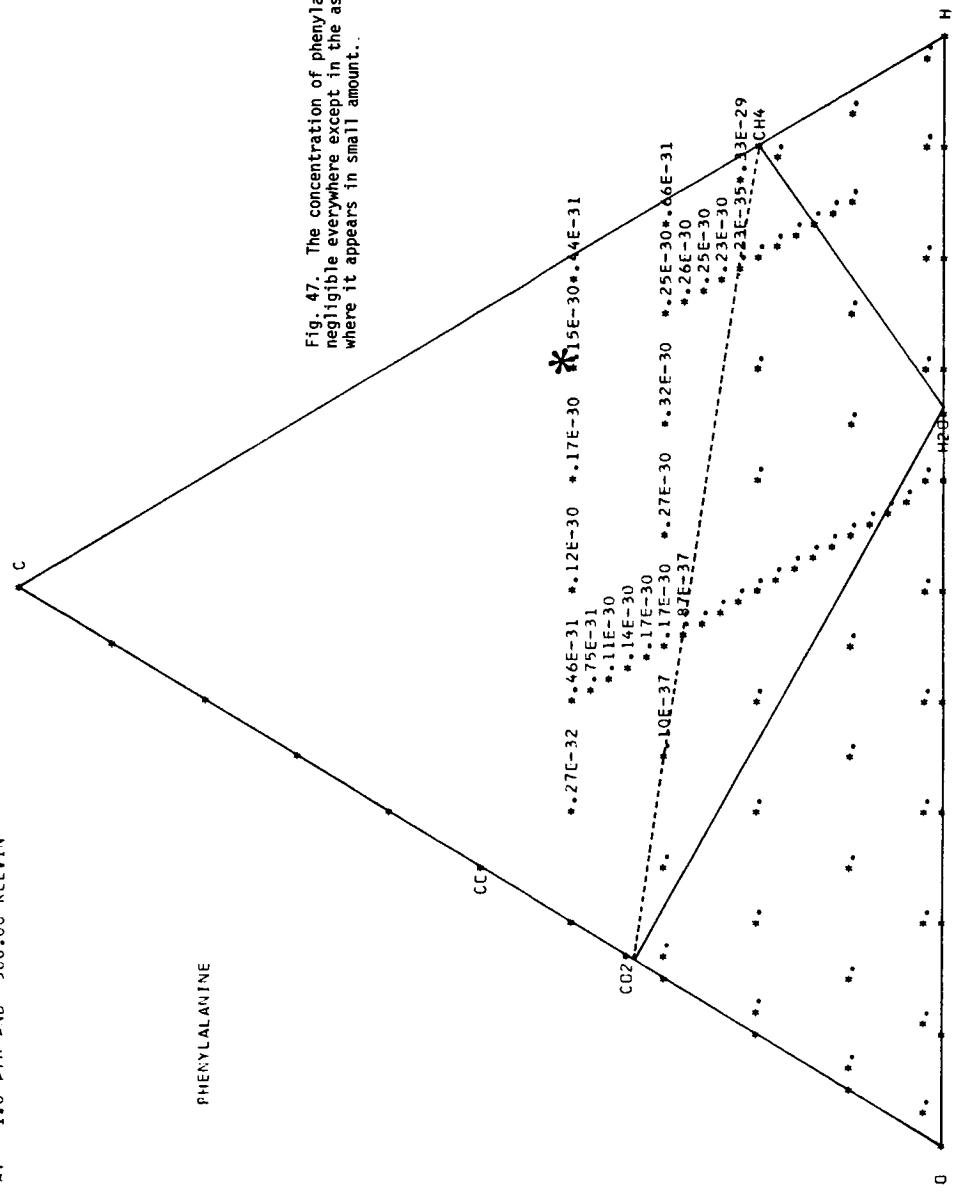


Fig. 47. The concentration of phenylalanine is negligible everywhere except in the asphalt region where it appears in small amount.

TABLE 3a

500°K AND 0.2 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{\partial G}{\partial n_i} / RT$ , FOR 68 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-98.160	-28.687	-0.837	-5.394	-159.832	-5.637	-98.273
2	2.0	9.0	89.0	-98.037	-27.895	-0.880	-5.376	-159.716	-5.888	-98.107
3	2.0	19.0	79.0	-97.831	-27.456	-0.956	-5.349	-159.513	-6.088	-97.825
4	2.0	29.0	69.0	-97.571	-27.165	-1.057	-5.319	-159.245	-6.237	-97.464
5	2.0	39.0	59.0	-97.218	-26.913	-1.202	-5.289	-158.866	-6.374	-96.965
6	2.0	49.0	49.0	-96.668	-26.645	-1.444	-5.256	-158.244	-6.536	-96.173
7	2.0	59.0	39.0	-95.345	-26.203	-2.070	-5.220	-156.661	-6.825	-94.217
8	2.0	69.0	29.0	-93.221	-2.276	-49.899	-5.210	-57.217	-30.697	-20.667
9	2.0	79.0	19.0	-7.572	-1.216	-52.578	-5.666	-53.233	-31.897	-22.930
10	2.0	89.0	9.0	-8.740	-0.955	-53.972	-6.179	-51.173	-32.285	-23.577
11	2.0	96.0	2.0	-9.237	-0.850	-55.770	-6.484	-48.496	-32.470	-23.865
12	10.0	2.0	88.0	-96.244	-28.589	-0.947	-5.351	-159.535	-5.607	-97.857
13	10.0	10.0	80.0	-96.047	-27.723	-1.023	-5.328	-159.334	-5.902	-97.583
14	10.0	20.0	70.0	-95.728	-27.281	-1.152	-5.298	-158.996	-6.118	-97.135
15	10.0	30.0	60.0	-95.257	-26.945	-1.355	-5.266	-158.473	-6.308	-96.462
16	10.0	40.0	50.0	-94.338	-26.554	-1.780	-5.231	-157.392	-6.568	-95.110
17	10.0	50.0	40.0	-0.689	-3.039	-48.632	-5.197	-59.117	-29.931	-19.142
18	10.0	60.0	30.0	-0.118	-2.804	-49.151	-5.160	-58.321	-30.090	-19.537
19	10.0	70.0	20.0	-0.327	-2.590	-49.639	-5.121	-57.568	-30.224	-19.883
20	10.0	80.0	10.0	-5.184	-1.354	-52.719	-5.393	-52.965	-31.535	-22.427
21	10.0	88.0	2.0	-6.636	-1.023	-55.123	-5.868	-49.391	-31.993	-23.218
22	20.0	2.0	78.0	-94.957	-28.411	-1.185	-5.292	-158.911	-5.580	-97.025
23	20.0	10.0	70.0	-94.564	-27.494	-1.355	-5.266	-158.472	-5.931	-96.462
24	20.0	20.0	60.0	-93.645	-26.900	-1.780	-5.231	-157.392	-6.280	-95.110
25	20.0	30.0	50.0	0.293	-3.277	-48.745	-5.195	-58.948	-29.692	-18.665
26	20.0	40.0	40.0	1.121	-3.109	-49.230	-5.156	-58.200	-29.780	-18.921
27	20.0	50.0	30.0	1.555	-3.055	-49.547	-5.112	-57.704	-29.750	-18.944
28	20.0	60.0	20.0	1.948	-3.039	-49.897	-5.065	-57.154	-29.670	-18.880
29	20.0	70.0	10.0	2.454	-3.073	-50.441	-5.011	-56.313	-29.530	-18.706
30	22.0	76.0	2.0	9.663	-4.806	-54.662	-5.755	-50.353	-29.284	-17.054
31	18.0	80.0	2.0	-1.685	-2.004	-52.727	-5.027	-52.876	-30.574	-20.818
32	30.0	2.0	68.0	-92.88C	-27.959	-1.953	-5.224	-156.958	-5.641	-94.578
33	30.0	10.0	60.0	2.142	-3.731	-49.456	-5.193	-57.881	-29.235	-17.754
34	30.0	20.0	50.0	7.243	-4.636	-52.038	-5.153	-53.988	-28.252	-16.160
35	30.0	30.0	40.0	9.859	-5.178	-53.414	-5.107	-51.901	-27.616	-16.179
36	30.0	40.0	30.0	9.845	-5.083	-53.498	-5.053	-51.748	-27.603	-16.046
37	30.0	50.0	20.0	9.822	-4.996	-53.630	-4.993	-51.521	-27.569	-15.875
38	30.0	60.0	10.0	9.796	-4.912	-53.897	-4.924	-51.086	-27.520	-15.631
39	30.0	68.0	2.0	9.774	-4.846	-54.638	-4.861	-49.943	-27.459	-15.253
40	40.0	10.0	50.0	10.345	-5.928	-53.528	-5.089	-51.721	-26.828	-16.260
41	40.0	20.0	40.0	10.096	-5.447	-53.458	-5.032	-51.797	-27.196	-16.099
42	40.0	30.0	30.0	9.599	-5.245	-53.491	-4.969	-51.717	-27.271	-15.925
43	40.0	40.0	20.0	9.934	-5.101	-53.589	-4.897	-51.534	-27.276	-15.721
44	40.0	50.0	10.0	9.880	-4.978	-53.826	-4.812	-51.136	-27.228	-15.439
45	40.0	58.0	2.0	9.840	-4.886	-54.540	-4.732	-50.024	-27.158	-15.000
46	12.0	78.0	10.0	-3.721	-1.648	-52.027	-5.195	-53.978	-31.136	-21.735
47	14.0	76.0	10.0	-0.397	-2.421	-50.433	-5.059	-56.343	-30.262	-20.090
48	16.0	74.0	10.0	0.782	-2.693	-50.135	-5.039	-56.784	-29.958	-19.516
49	18.0	72.0	10.0	1.530	-2.861	-50.183	-5.025	-56.705	-29.767	-19.156
50	22.0	68.0	10.0	8.198	-4.491	-53.168	-4.998	-52.215	-28.085	-16.038
51	24.0	66.0	10.0	9.706	-4.872	-53.908	-4.981	-51.097	-27.670	-15.730
52	26.0	64.0	10.0	9.748	-4.888	-53.911	-4.963	-51.084	-27.617	-15.698
53	28.0	62.0	10.0	9.775	-4.901	-53.906	-4.944	-51.082	-27.566	-15.665
54	4.0	56.0	40.0	-94.330	-26.147	-2.228	-5.217	-156.266	-6.874	-93.738
55	6.0	54.0	40.0	-92.499	-25.805	-2.933	-5.209	-154.498	-7.201	-91.606
56	8.0	52.0	40.0	-1.380	-3.123	-48.371	-5.204	-59.513	-29.861	-18.989
57	12.0	48.0	40.0	-0.254	-3.019	-48.776	-5.189	-58.898	-29.936	-19.167
58	14.0	46.0	40.0	0.106	-3.022	-48.890	-5.181	-58.724	-29.918	-19.145
59	16.0	44.0	40.0	0.438	-3.039	-48.996	-5.173	-58.561	-29.885	-19.096
60	18.0	42.0	40.0	0.769	-3.067	-49.106	-5.164	-58.391	-29.840	-19.022
61	22.0	38.0	40.0	1.523	-3.169	-49.383	-5.146	-57.967	-29.704	-18.783
62	24.0	36.0	40.0	2.032	-3.261	-49.592	-5.137	-57.648	-29.594	-18.582
63	26.0	34.0	40.0	2.827	-3.427	-49.946	-5.128	-57.113	-29.410	-18.232
64	28.0	32.0	40.0	7.464	-4.456	-52.226	-5.119	-53.689	-28.263	-16.215
65	32.0	28.0	40.0	9.916	-5.218	-53.428	-5.093	-51.872	-27.547	-16.167
66	34.0	26.0	40.0	9.959	-5.261	-53.436	-5.078	-51.854	-27.477	-16.150
67	36.0	24.0	40.0	10.000	-5.309	-53.441	-5.063	-51.838	-27.397	-16.132
68	38.0	22.0	40.0	10.044	-5.369	-53.448	-5.048	-51.821	-27.308	-16.114

TABLE 3b

500°K AND 0.2 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

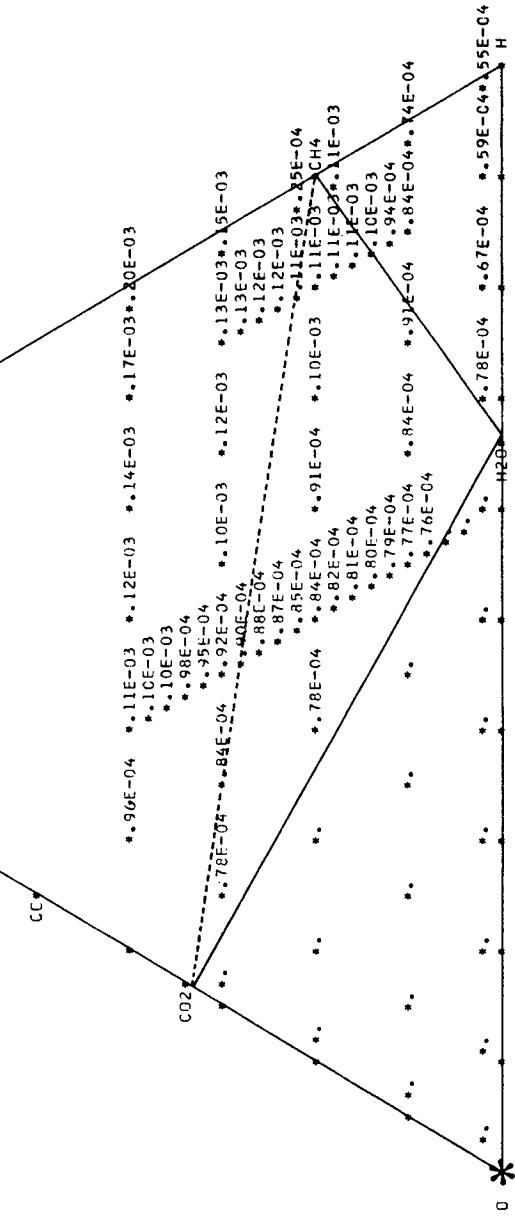
COMPOUND	A	B	C	D	E	F	G
METHANE	3.5E-02	1.6E-01	2.6E-01	3.3E-01	7.2E-01	7.1E-01	0.
H2	1.1E-02	1.0E-02	1.6E-04	3.0E-01	1.1E-02	2.7E-04	1.0E-23
O2	0.	0.	0.	0.	0.	0.	5.0E-01
WATER	6.8E-01	3.3E-01	7.9E-05	3.3E-01	1.0E-01	8.3E-05	2.5E-01
CO	3.4E-05	1.2E-04	1.1E-02	6.4E-09	1.3E-04	6.4E-03	7.6E-26
CO2	2.7E-01	5.0E-01	7.2E-01	8.5E-07	1.7E-01	2.6E-01	2.5E-01
BENZENE	6.7E-27	2.3E-22	5.5E-05	3.2E-34	8.4E-19	1.9E-04	0.
NAPHTHALENE	0.	5.2E-36	3.0E-05	0.	4.3E-30	1.3E-04	0.
ASPHALT	0.	0.	4.5E-03	0.	0.	2.7E-02	0.
N2	1.5E-04	1.7E-04	1.8E-04	1.0E-04	2.2E-04	2.6E-04	1.3E-04
NH3	9.9E-07	8.4E-07	1.8E-09	1.3E-04	1.1E-06	4.7E-09	2.3E-38
HCN	1.0E-15	5.9E-15	4.9E-12	4.9E-17	2.7E-14	7.2E-12	0.
NO	3.4E-32	2.0E-32	3.1E-34	4.7E-34	6.7E-33	2.3E-34	1.3E-11
NO2	0.	0.	0.	0.	0.	0.	4.8E-10
N2O	4.0E-38	2.4E-38	0.	0.	9.4E-39	0.	1.4E-17
NITRIOUS ACID	0.	0.	0.	0.	0.	0.	4.2E-13
NITRIC ACID	0.	0.	0.	0.	0.	0.	2.7E-12
C2N2	2.3E-35	9.3E-34	4.0E-26	0.	1.8E-32	5.0E-26	0.
HNCC	1.7E-14	5.6E-14	7.1E-13	1.4E-17	7.6E-14	6.4E-13	0.
P2	0.	0.	0.	0.	0.	0.	0.
P4O6	7.7E-05	8.4E-05	9.2E-05	8.4E-05	1.1E-04	1.3E-04	0.
P4O10	1.3E-37	1.3E-38	0.	0.	0.	0.	6.3E-05
PO	2.9E-36	4.0E-36	3.3E-35	2.3E-35	7.8E-36	4.6E-35	0.
PO2	9.7E-31	7.3E-31	9.3E-32	1.3E-31	4.3E-31	8.0E-32	7.1E-33
PH2	3.8E-30	8.2E-30	7.2E-29	5.2E-26	5.9E-29	2.8E-28	0.
PH3	8.6E-28	1.8E-27	1.9E-27	6.4E-23	1.3E-26	9.6E-27	0.
PCL3	7.2E-35	2.8E-34	1.0E-28	2.7E-34	3.9E-33	3.0E-28	0.
POCL3	2.7E-31	5.8E-31	3.2E-27	1.7E-32	2.4E-30	5.9E-27	5.0E-23
PSCL3	1.9E-30	9.5E-30	5.3E-23	2.8E-31	1.6E-28	2.8E-22	0.
CL2	5.0E-26	6.8E-26	5.2E-24	2.0E-27	1.1E-25	6.2E-24	2.4E-05
HCl	3.1E-04	3.4E-04	3.7E-04	3.4E-04	4.5E-04	5.3E-04	2.0E-04
HOCl	4.0E-28	2.4E-28	4.0E-30	7.3E-30	9.4E-29	3.5E-30	1.1E-07
CL2C	0.	0.	0.	0.	0.	0.	7.3E-17
CH3Cl	1.4E-12	8.1E-12	8.9E-10	5.0E-13	4.4E-11	2.0E-09	0.
CH2Cl2	6.3E-24	4.5E-23	3.4E-19	8.3E-26	3.0E-22	6.6E-19	0.
CHCl3	1.8E-35	1.6E-34	8.2E-29	8.6E-39	1.3E-33	1.3E-28	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
COCl2	6.5E-27	2.9E-26	2.1E-22	4.9E-32	5.5E-26	1.5E-22	6.9E-27
S2	1.2E-16	1.8E-16	4.4E-14	1.7E-19	2.8E-16	1.3E-13	0.
S8	0.	0.	5.9E-38	0.	0.	4.8E-36	0.
H2S	3.1E-04	3.4E-04	8.4E-05	3.4E-04	4.5E-04	2.5E-04	0.
S02	1.5E-16	5.6E-17	2.0E-19	1.6E-21	6.2E-18	1.3E-19	3.5E-09
S03	2.6E-32	5.4E-33	2.9E-37	0.	1.8E-34	1.2E-37	2.5E-04
COS	4.6E-08	1.9E-07	2.9E-04	3.3E-13	2.7E-07	2.9E-04	0.
CS2	1.8E-15	1.7E-14	2.6E-08	2.8E-20	1.0E-13	7.2E-08	0.
SU	1.1E-22	7.7E-23	1.8E-23	7.1E-26	2.9E-23	2.0E-23	6.3E-36
SULFURIC ACID	8.3E-38	1.5E-38	0.	0.	0.	0.	7.2E-31
SULFURIC ACID	0.	0.	0.	0.	0.	0.	3.4E-13
CYANODISULFIDE	0.	1.8E-37	1.2E-28	0.	4.3E-36	2.6E-28	0.
METHANETHIOL	1.5E-11	8.7E-11	2.2E-09	5.4E-12	4.7E-10	1.0E-08	0.
DIMETHYLSULFIDE	1.5E-18	4.6E-17	1.1E-13	1.7E-19	1.0E-15	8.5E-13	0.
DIMET.DISULFIDE	8.4E-25	3.2E-23	1.2E-18	3.6E-27	8.8E-22	1.6E-17	0.
ETHANETHIOL	4.1E-17	1.2E-15	3.1E-12	4.7E-18	2.8E-14	2.3E-11	0.
DIETHYLSULFIDE	9.8E-30	8.4E-27	2.1E-19	1.2E-31	3.1E-24	3.9E-18	0.
DIETH.DISULFIDE	1.0E-35	1.1E-32	4.1E-24	0.	4.9E-30	1.4E-22	0.
OCTANETHIOL	1.1E-26	4.2E-25	1.6E-20	4.8E-29	1.2E-23	2.1E-19	0.
THIOCFCRIC ACID	7.4E-26	2.7E-25	6.3E-24	1.5E-29	4.0E-25	1.1E-23	0.
THICACETIC ACID	2.4E-29	4.7E-28	1.1E-24	1.6E-33	2.9E-27	3.0E-24	0.
CYCLOPROP.C.ICL	6.1E-26	1.1E-23	1.7E-16	7.8E-29	9.5E-22	1.2E-15	0.
CYCLOPUA.THICL	1.5E-32	1.4E-29	2.2E-20	6.0E-36	4.9E-27	2.5E-19	0.
CYCLOPENT.THICL	1.8E-34	9.2E-31	1.4E-19	2.4E-38	1.3E-27	2.5E-18	0.
CYCLOHEXA.THICL	7.5E-38	2.1E-33	3.2E-20	0.	1.2E-29	9.2E-19	0.
M-SULFONIC ACID	5.2E-38	5.0E-38	0.	0.	7.2E-39	0.	0.
E-SULFINIC ACID	3.4E-14	5.7E-13	2.1E-11	6.5E-17	3.8E-12	9.9E-11	0.
THIOPHENE	1.7E-26	2.2E-23	1.3E-10	8.3E-33	6.5E-21	5.2E-10	0.
BENZENETHIOL	7.8E-34	3.3E-29	1.2E-10	0.	1.5E-25	7.2E-10	0.
THIOCYANIC ACID	9.3E-22	6.9E-21	8.8E-17	1.7E-24	3.9E-20	2.3E-16	0.
THICGLYCOL	2.0E-32	3.4E-31	1.3E-29	3.9E-35	2.3E-30	6.0E-29	0.
CYSTEINE	0.	2.0E-38	9.3E-36	0.	1.8E-37	3.9E-35	0.
METHICNINE	0.	0.	0.	0.	0.	0.	0.

AT C.2 ATM AND 500.00 KELVIN

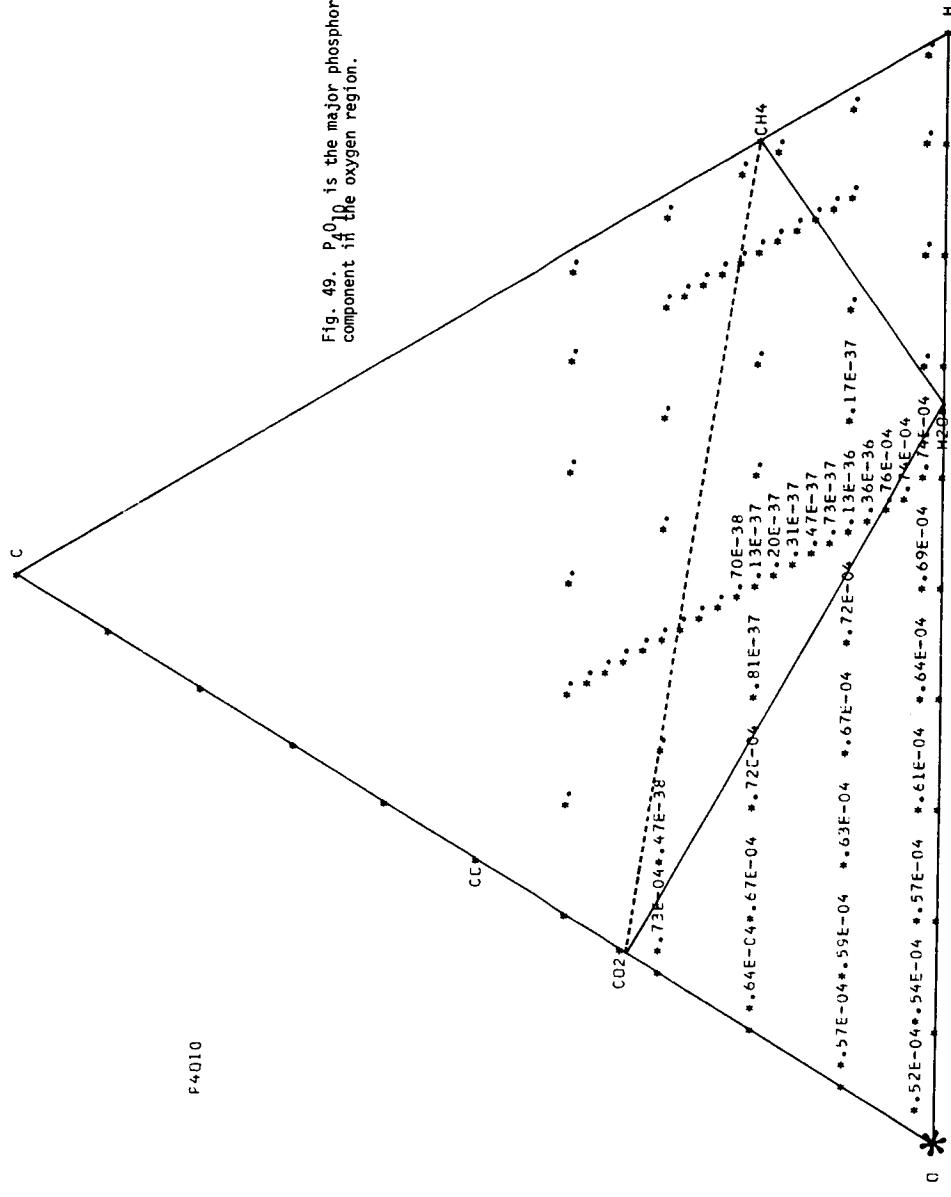
C

P406

Fig. 48.  $P_4O_6$  is the major phosphorus containing species everywhere except in the oxygen region.



AT C.2 ATM AND 5000.00 KELVIN

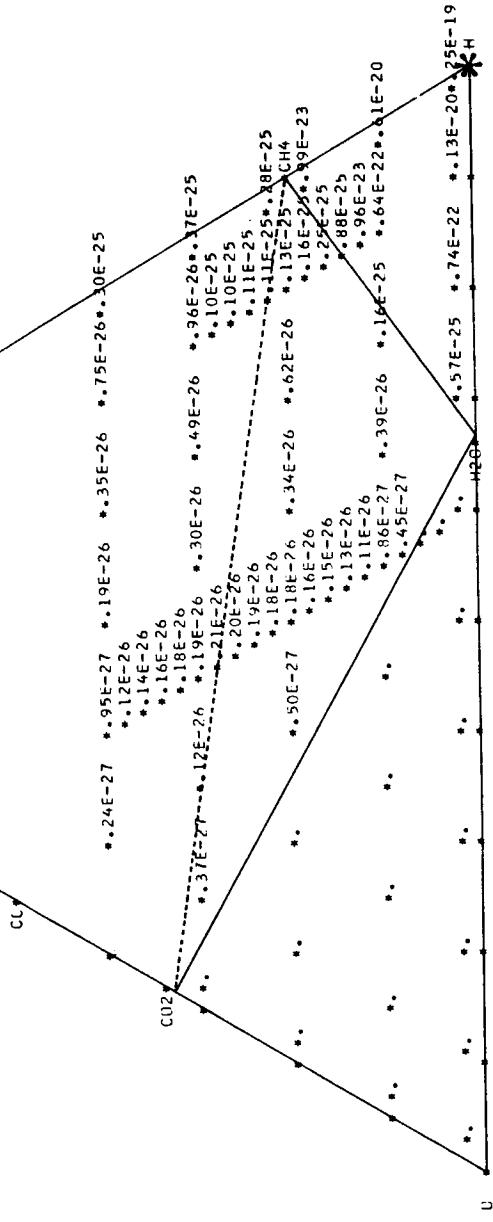


AT C=2 ATM AND 500.0C KELVIN

C

PH3

Fig. 50b. The concentration of phosphine is negligible in the oxygen region and very low in the other regions.



AT C\*2 ATM AND 500.0 CC KELVIN

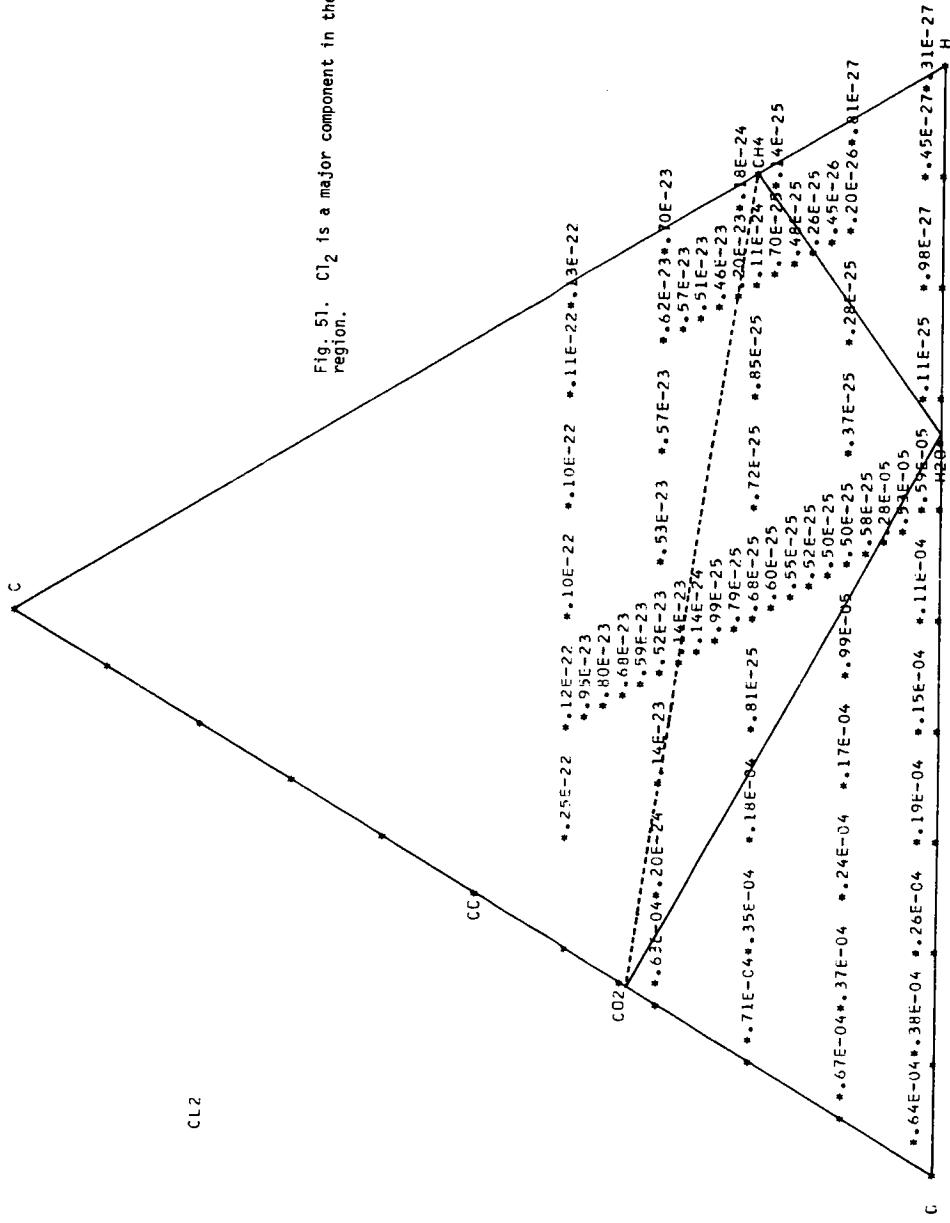


Fig. 51. Cl<sub>2</sub> is a major component in the oxygen region.

AT 0.2 ATM AND 500.0°C KELVIN

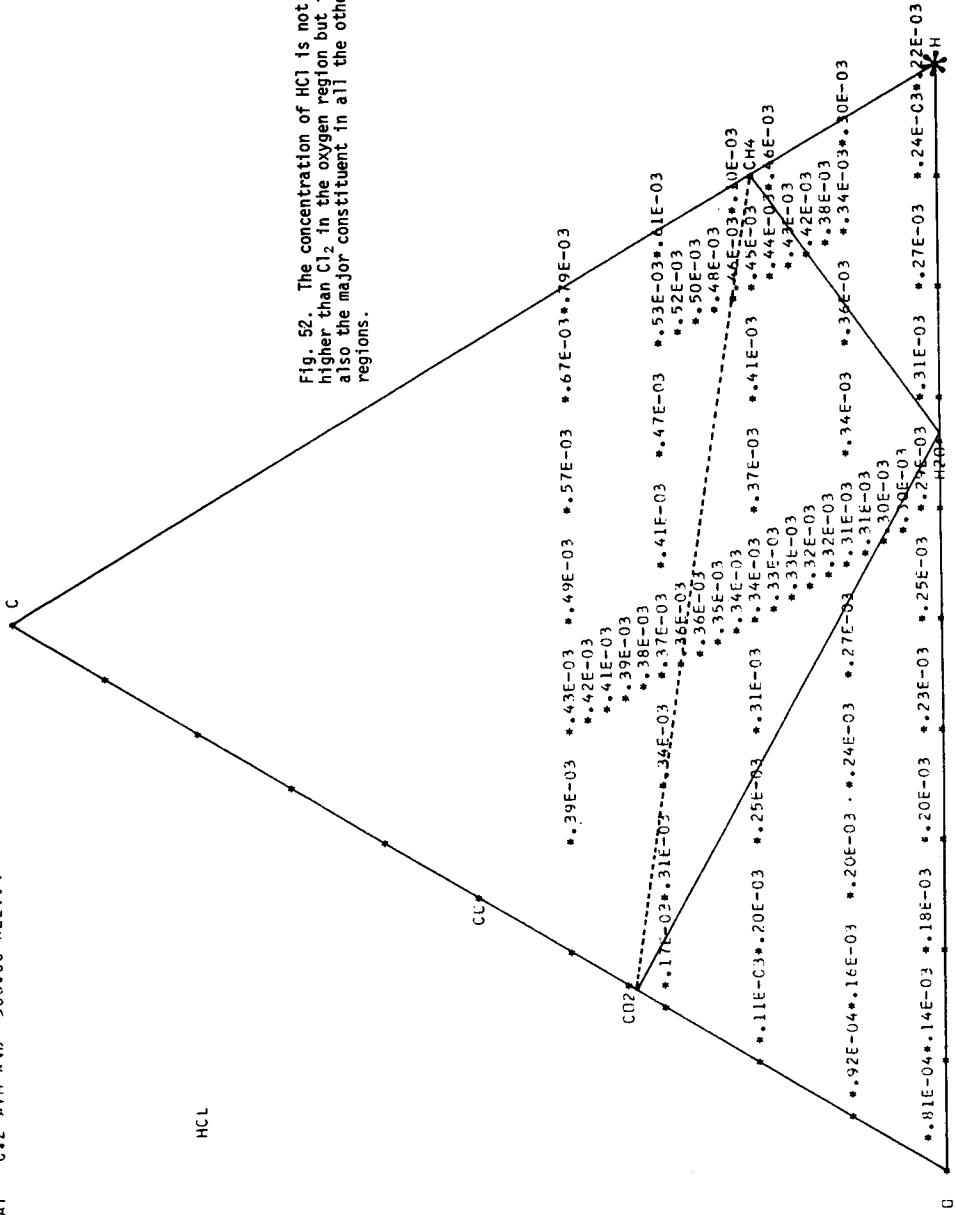


Fig. 52. The concentration of HCl is not only higher than Cl<sub>2</sub> in the oxygen region but it is also the major constituent in all the other regions.

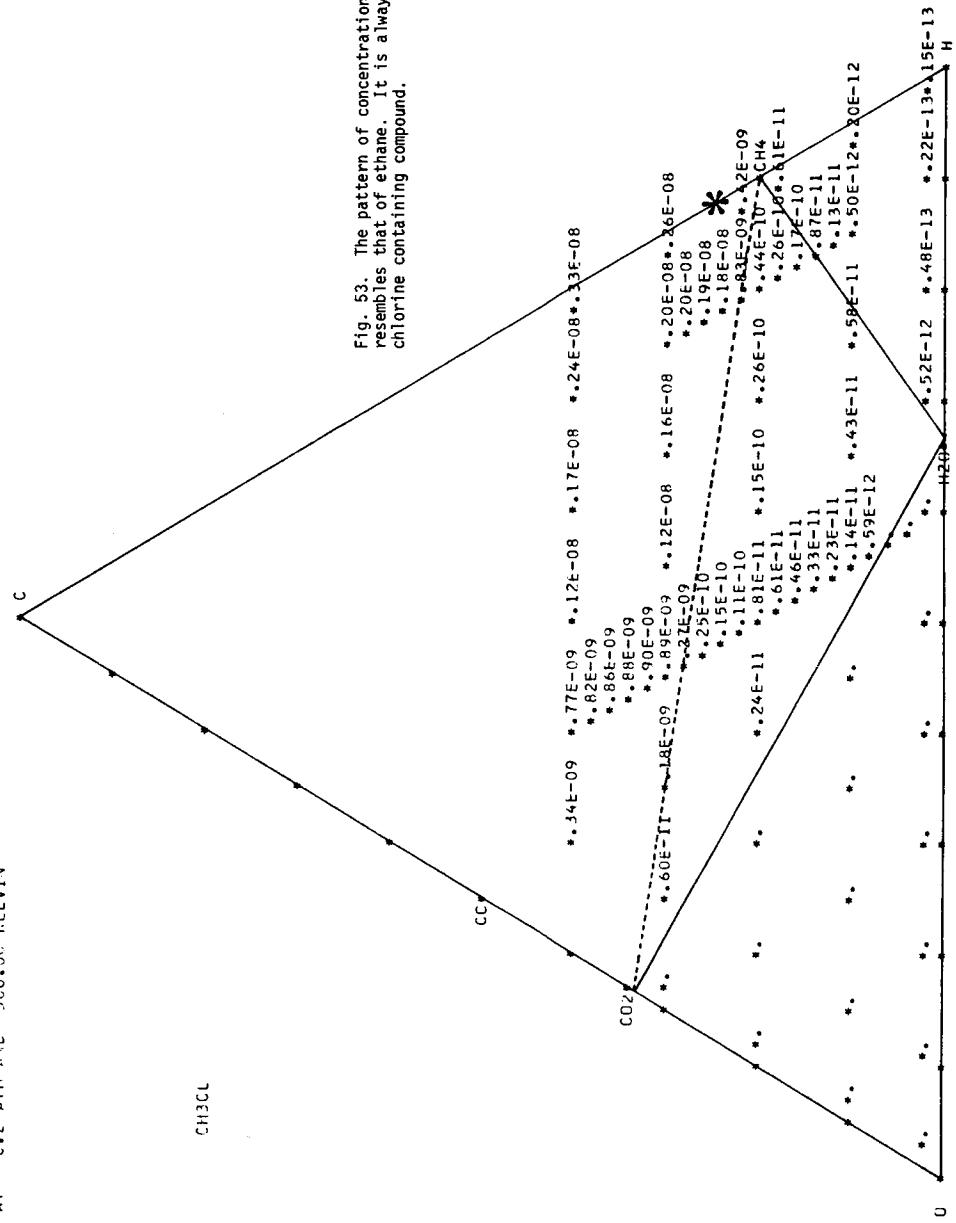


Fig. 53. The pattern of concentrations of  $\text{CH}_3\text{Cl}$  resembles that of ethane. It is always a minor chlorine containing compound.

AT 0.2 ATM AND 500.00 KELVIN

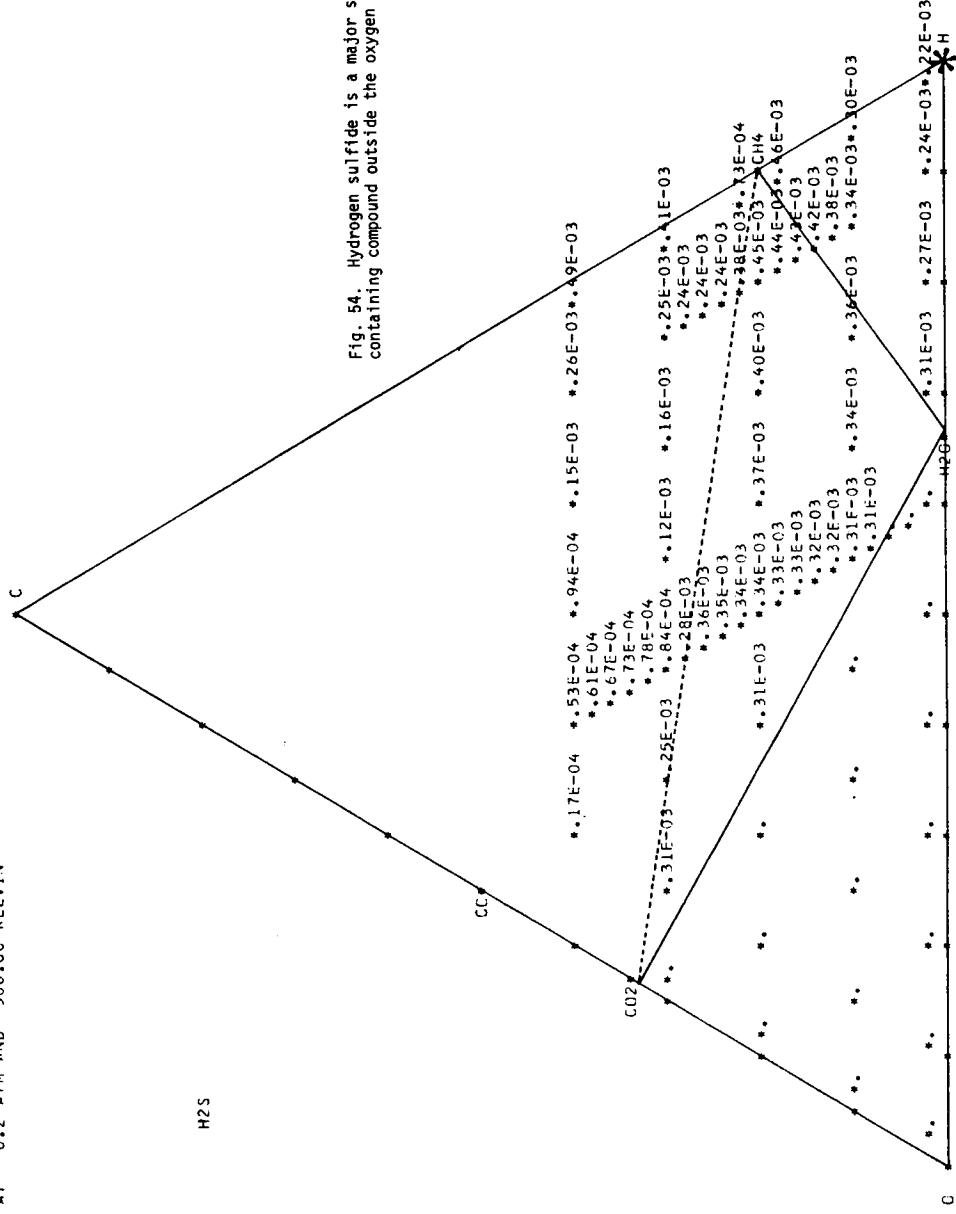


Fig. 54. Hydrogen sulfide is a major sulfur containing compound outside the oxygen region.

AT C\*2 ATM ANC 500.CC KELVIN

S02

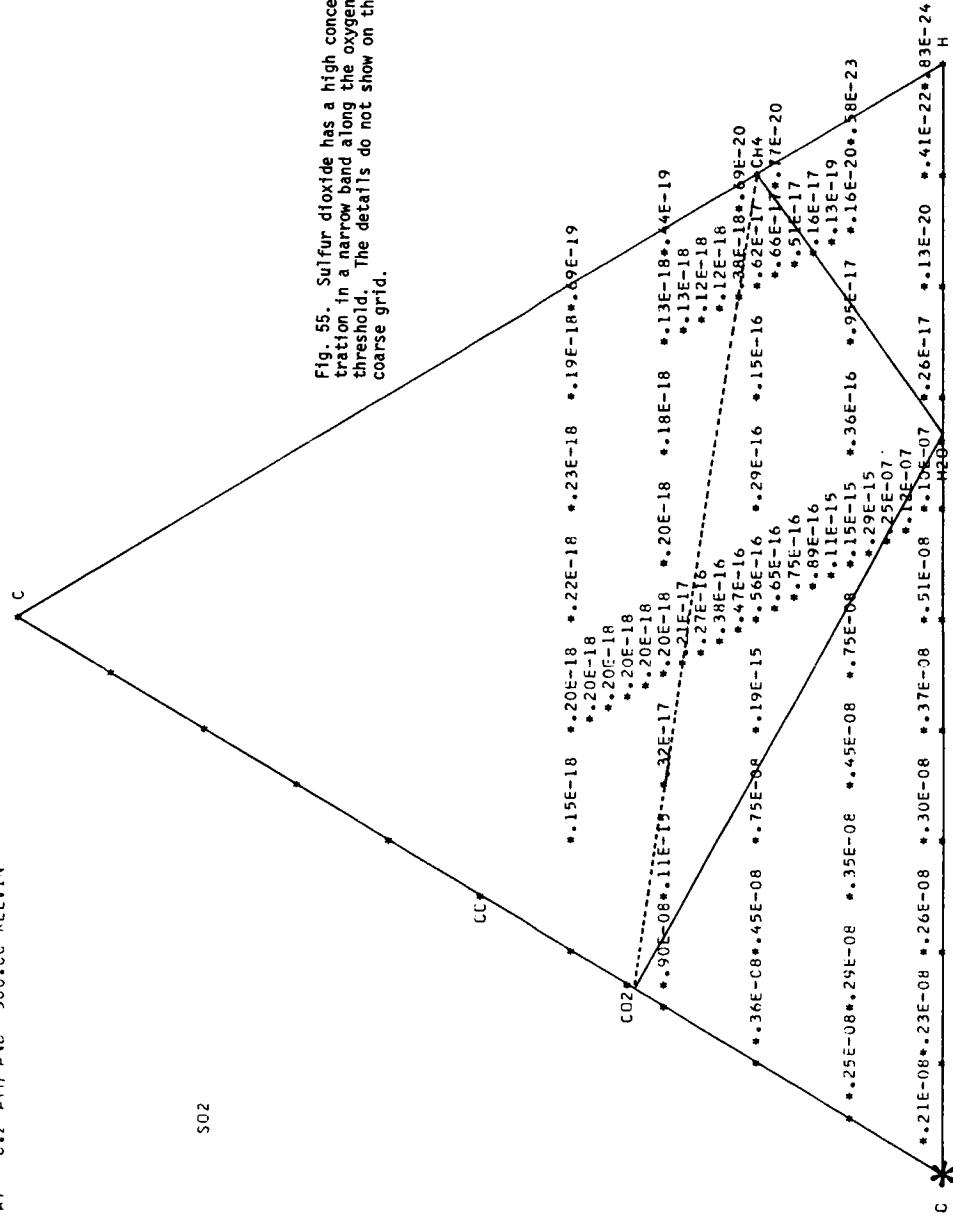


Fig. 55. Sulfur dioxide has a high concentration in a narrow band along the oxygen threshold. The details do not show on this coarse grid.

AT C=2 ATM AND 500°CC KELVIN

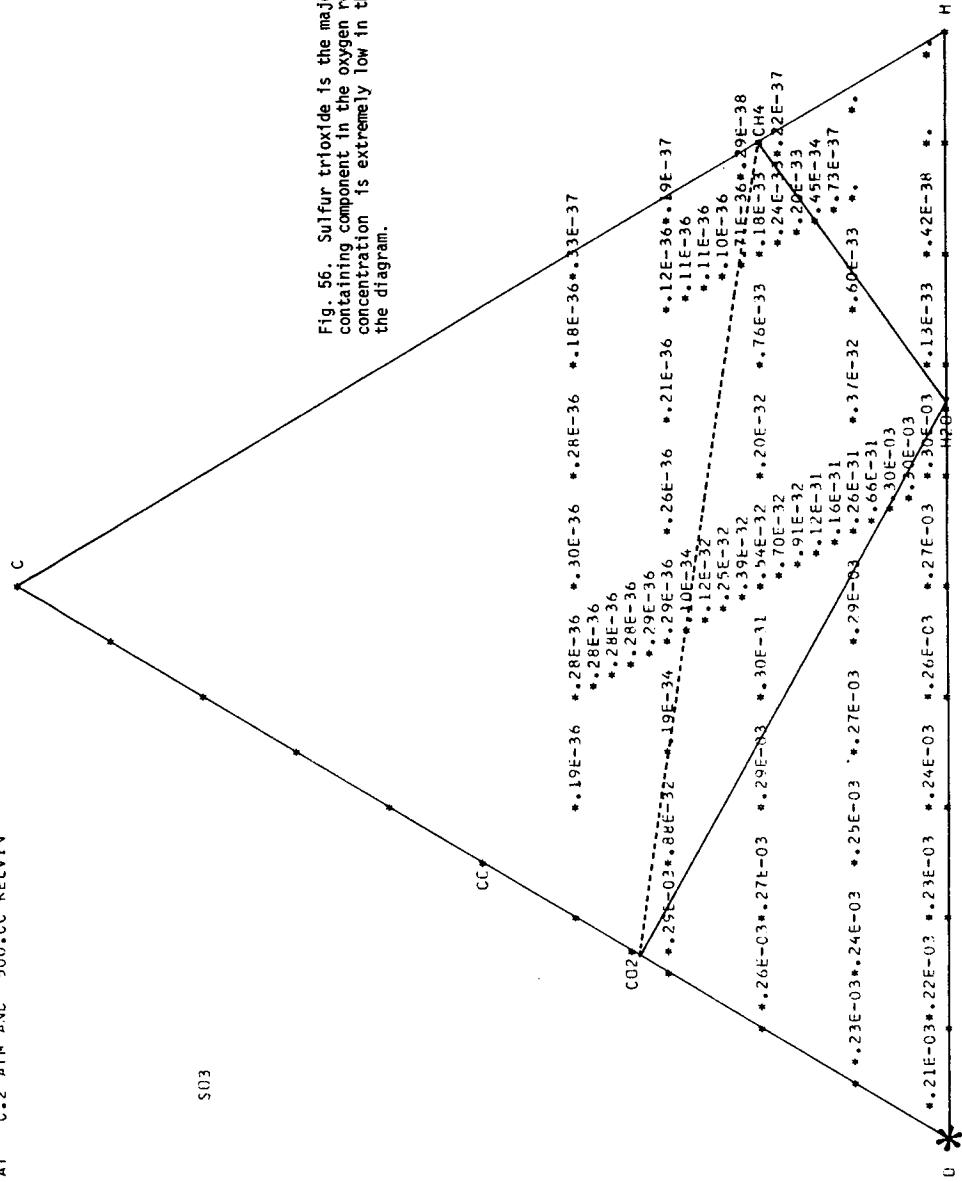


Fig. 56. Sulfur trioxide is the major sulfur containing component in the oxygen region. Its concentration is extremely low in the rest of the diagram.

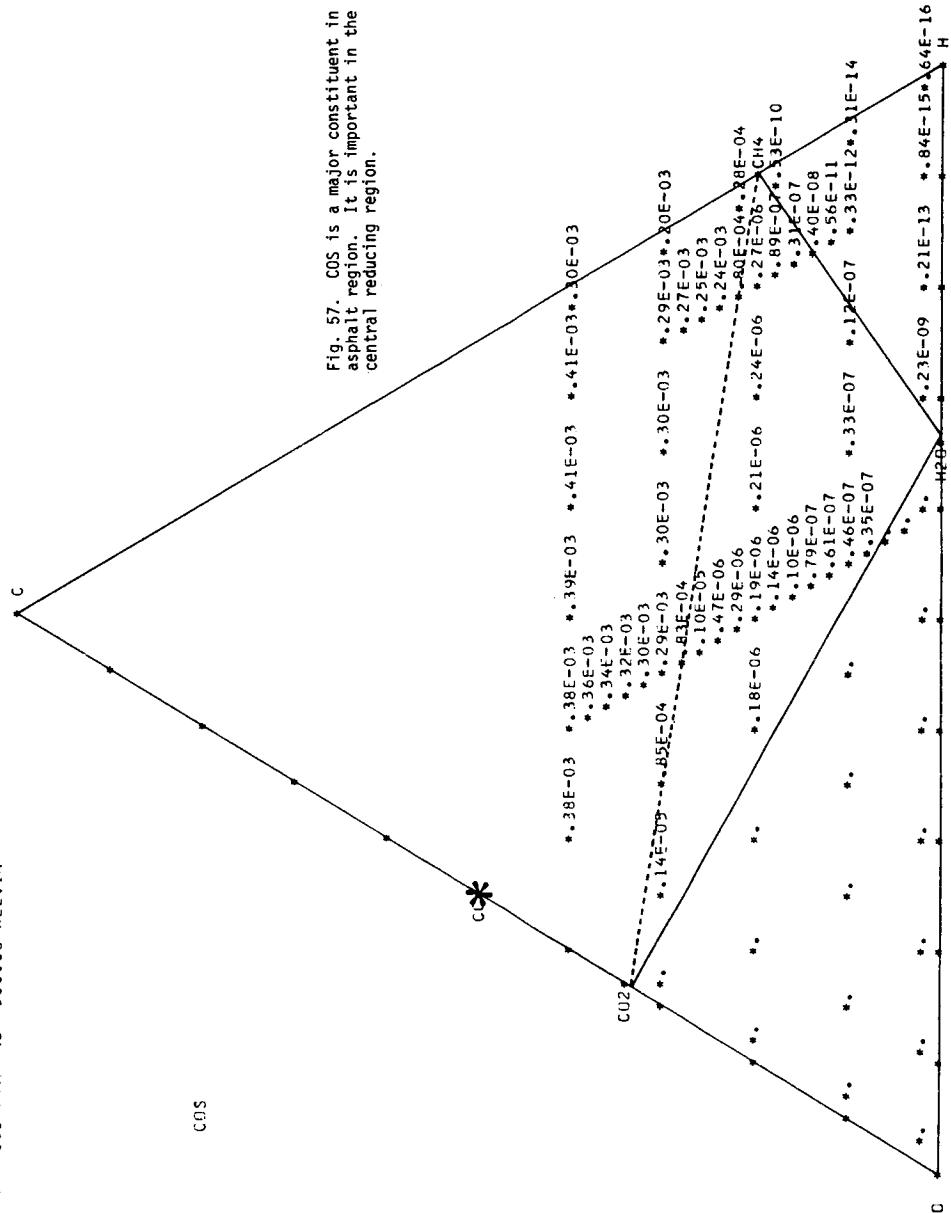


Fig. 57. COS is a major constituent in the asphalt region. It is important in the central reducing region.

AT C.2 ATM AND 500.0C KELVIN

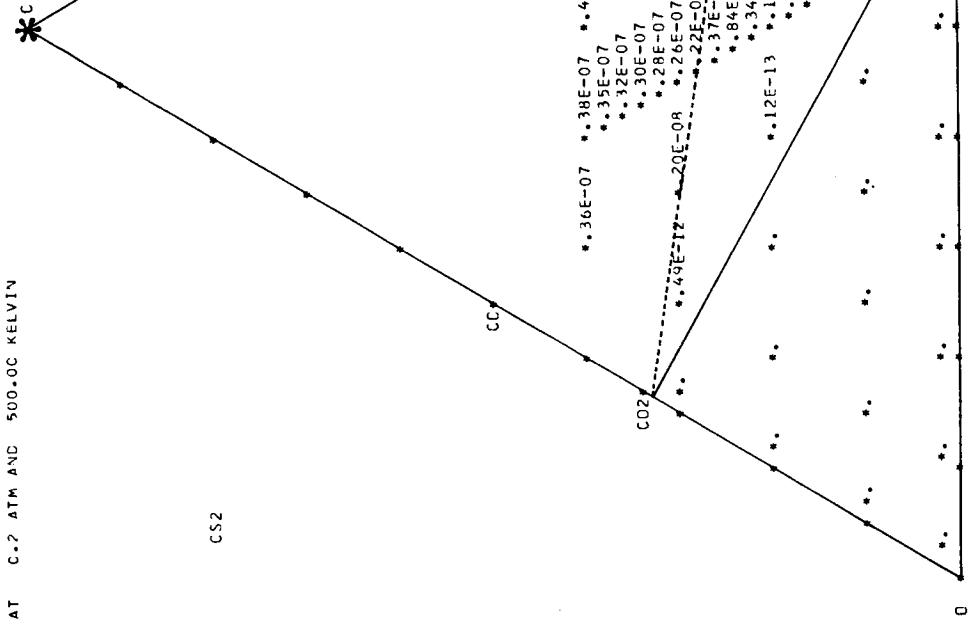


Fig. 58. CS<sub>2</sub> is most concentrated in the asphalt region. For systems containing more sulfur, it would be a major constituent here.

AT C.2 ATM AND 500.0C KELVIN

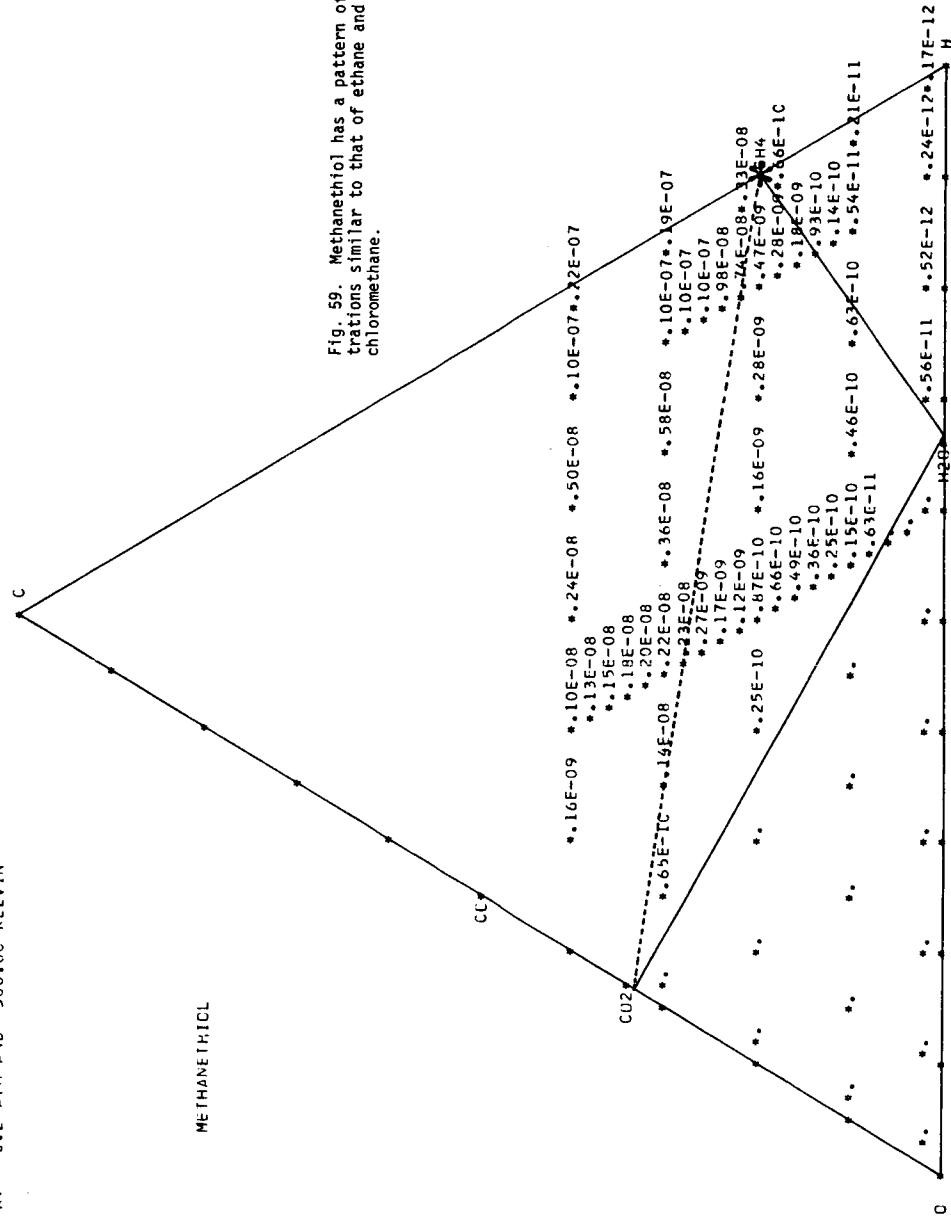


Fig. 59. Methanethiol has a pattern of concentrations similar to that of ethane and chloromethane.

AT C.2 ATM AND 500.00 KELVIN

BENZENETHIOL

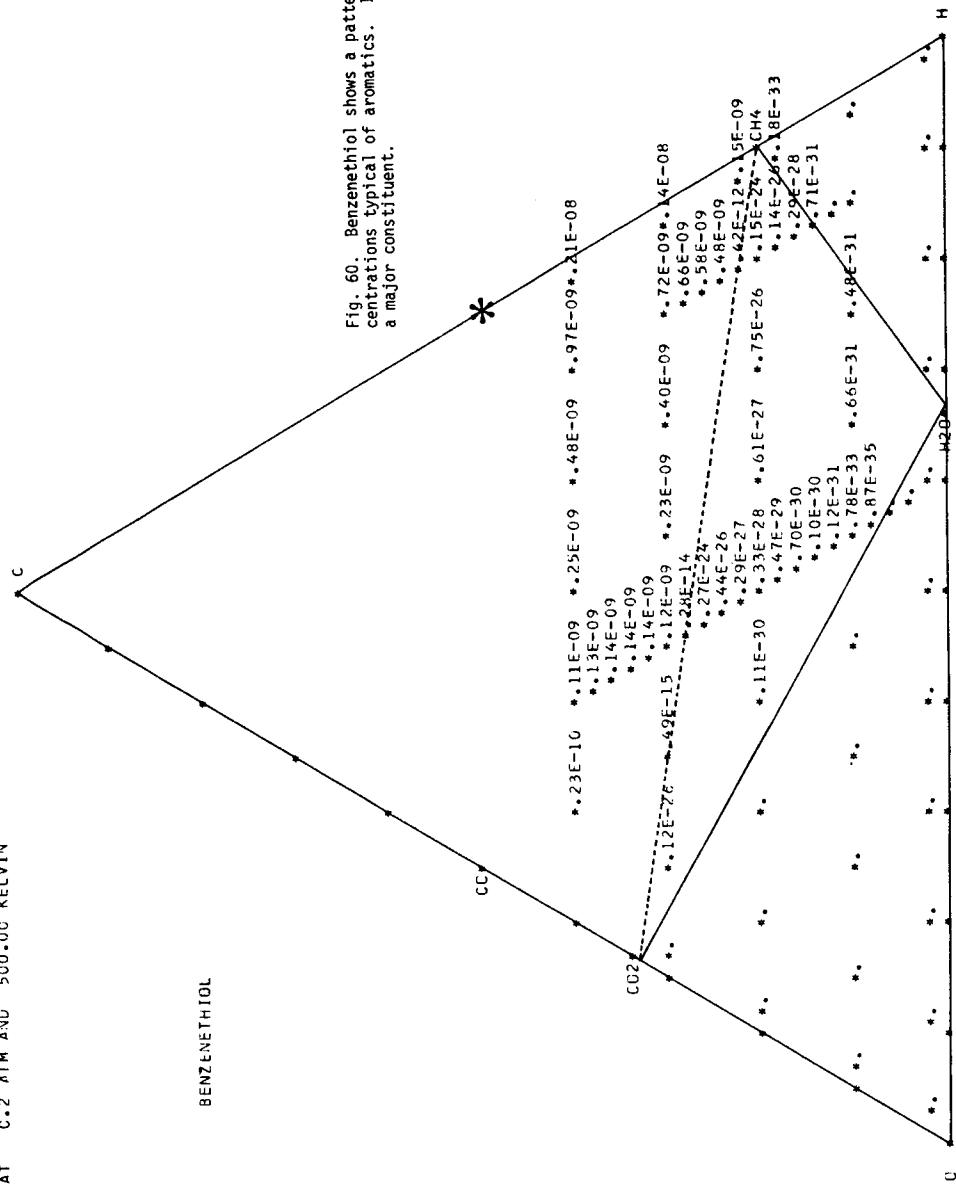


Fig. 60. Benzenethiol shows a pattern of concentrations typical of aromatics. It is never a major constituent.

AT C•2 ATM AND 500•00 KELVIN

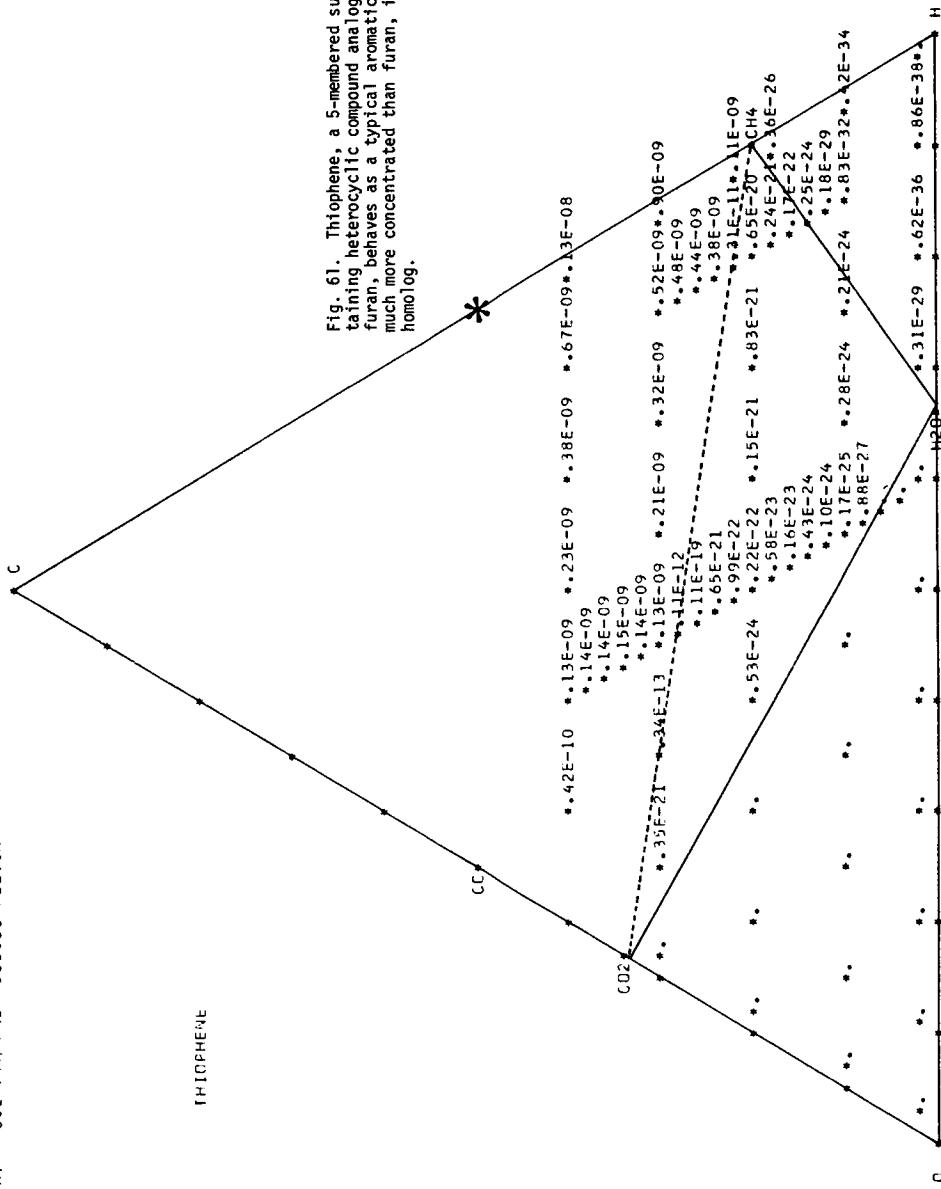
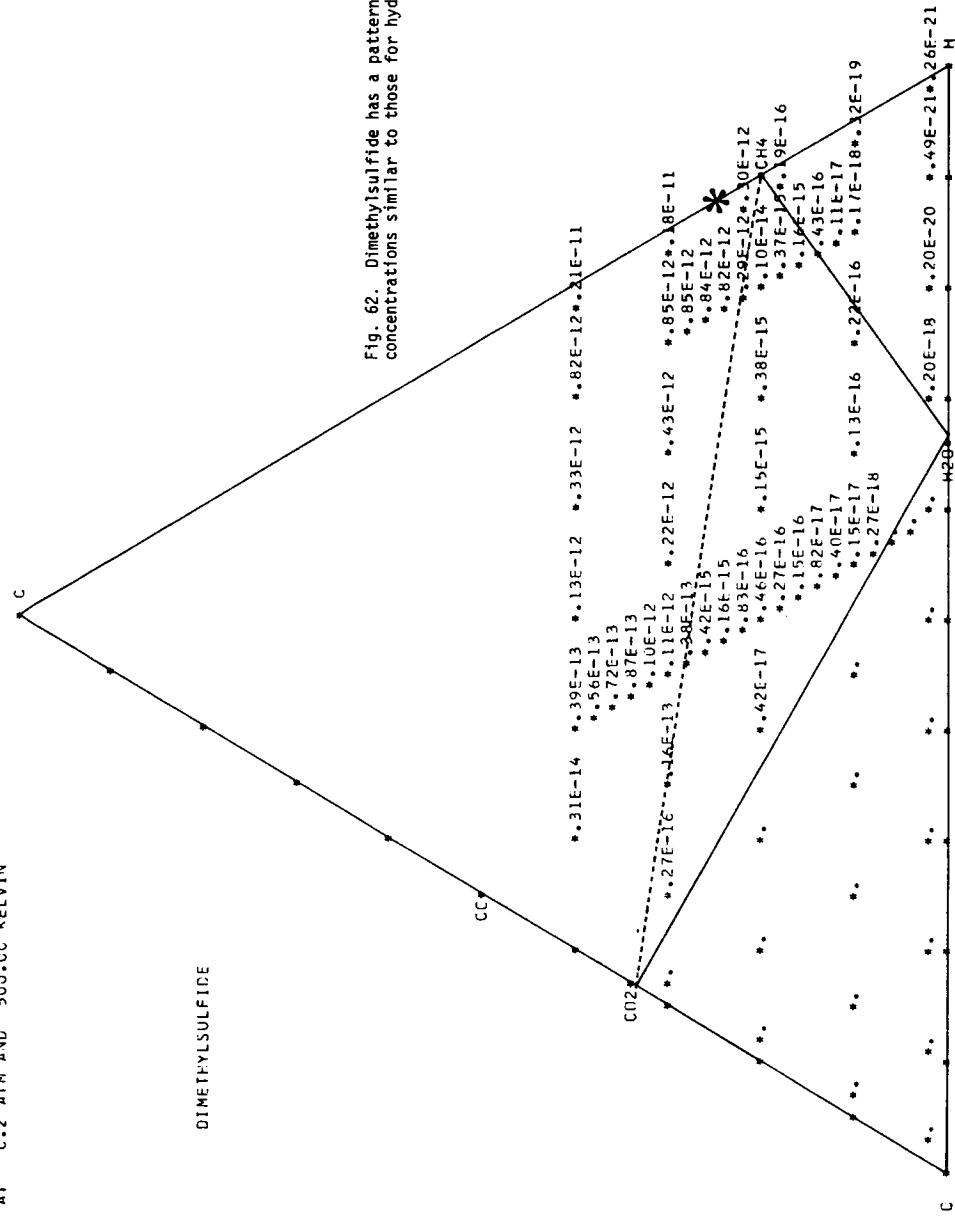


Fig. 61. Thiophene, a 5-membered sulfur containing heterocyclic compound analogous to furan, behaves as a typical aromatic. It is much more concentrated than furan, its oxygen homolog.

AT C=2 ATM AND 500.00 KELVIN



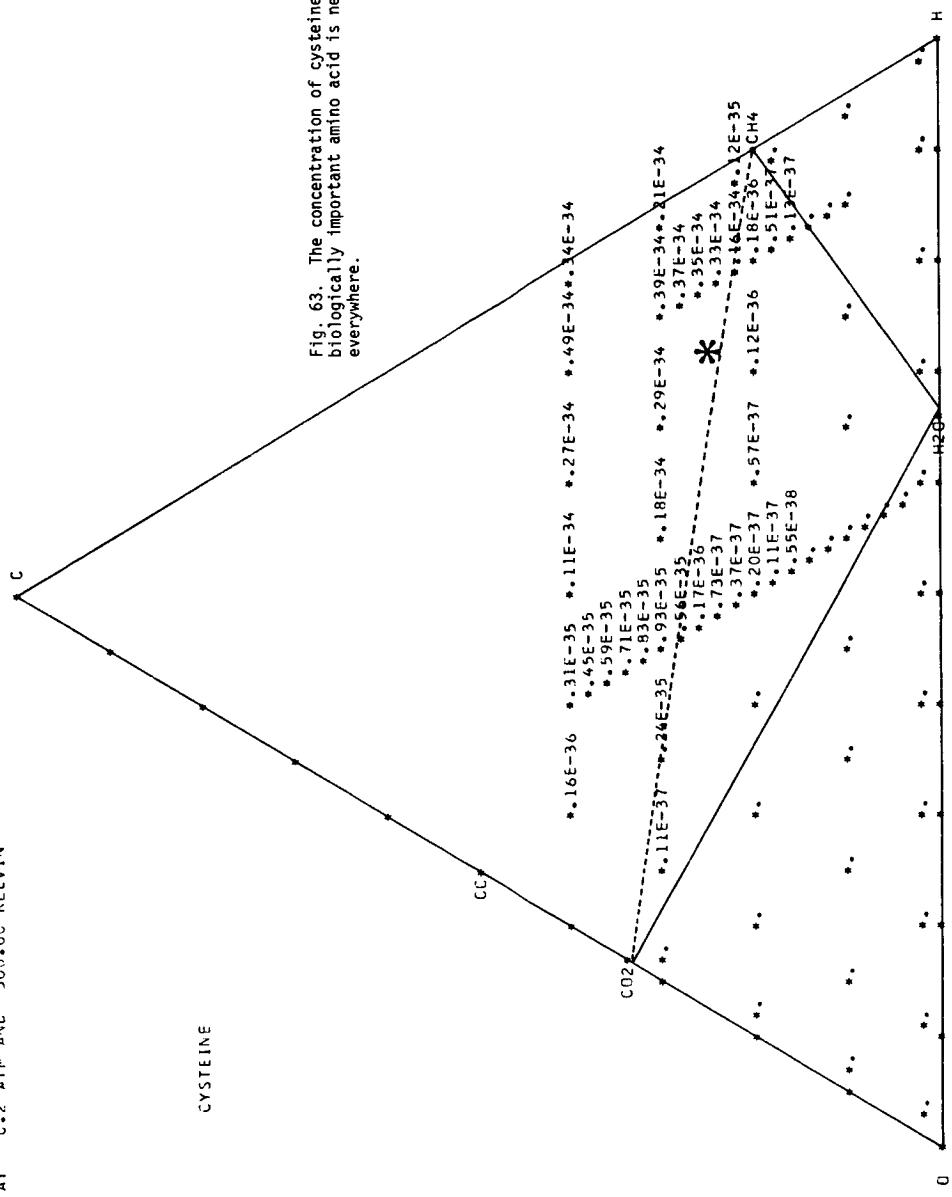


Fig. 63. The concentration of cysteine, a biologically important amino acid is negligible everywhere.

TABLE 4a

300°K AND  $1 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  
 $\bar{F}_j/RT$ , FOR 45 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL  
 NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-161.300	-49.880	-4.303	-3.562
2	2.0	9.0	89.0	-161.177	-49.096	-4.361	-3.559
3	2.0	19.0	79.0	-160.971	-48.668	-4.459	-3.554
4	2.0	29.0	69.0	-160.711	-48.389	-4.583	-3.549
5	2.0	39.0	59.0	-160.358	-48.150	-4.754	-3.543
6	2.0	49.0	49.0	-159.809	-47.896	-5.024	-3.538
7	2.0	59.0	39.0	-158.493	-47.472	-5.676	-3.533
8	2.0	69.0	29.0	-7.932	-6.013	-88.603	-3.529
9	2.0	79.0	19.0	-12.442	-4.889	-91.287	-3.538
10	2.0	89.0	9.0	-13.606	-4.600	-92.620	-3.546
11	2.0	96.0	2.0	-14.116	-4.474	-94.382	-3.552
12	10.0	2.0	88.0	-159.384	-49.799	-4.448	-3.554
13	10.0	10.0	80.0	-159.187	-48.963	-4.542	-3.550
14	10.0	20.0	70.0	-158.869	-48.515	-4.696	-3.545
15	10.0	30.0	60.0	-158.399	-48.192	-4.926	-3.540
16	10.0	40.0	50.0	-157.482	-47.816	-5.379	-3.535
17	10.0	50.0	40.0	0.473	-8.233	-84.418	-3.529
18	10.0	60.0	30.0	1.006	-8.016	-84.958	-3.524
19	10.0	70.0	20.0	0.730	-7.805	-85.505	-3.518
20	10.0	80.0	10.0	-9.930	-5.107	-91.463	-3.523
21	10.0	88.0	2.0	-11.368	-4.750	-93.796	-3.530
22	20.0	2.0	78.0	-158.098	-49.646	-4.734	-3.544
23	20.0	10.0	70.0	-157.705	-48.741	-4.926	-3.540
24	20.0	20.0	60.0	-156.789	-48.163	-5.379	-3.535
25	20.0	30.0	50.0	1.443	-8.474	-84.522	-3.529
26	20.0	40.0	40.0	2.247	-8.326	-85.030	-3.524
27	20.0	50.0	30.0	2.671	-8.290	-85.381	-3.518
28	20.0	60.0	20.0	3.054	-8.293	-85.769	-3.513
29	20.0	70.0	10.0	3.530	-8.344	-86.348	-3.507
30	22.0	76.0	2.0	15.920	-11.076	-92.543	-3.657
31	18.0	80.0	2.0	-6.328	-5.853	-91.550	-3.506
32	30.0	2.0	68.0	-156.027	-49.224	-5.556	-3.533
33	30.0	10.0	60.0	3.266	-8.930	-85.220	-3.529
34	30.0	20.0	50.0	15.772	-11.708	-91.537	-3.524
35	30.0	30.0	40.0	16.226	-11.730	-91.870	-3.518
36	30.0	40.0	30.0	16.220	-11.661	-92.005	-3.512
37	30.0	50.0	20.0	16.208	-11.603	-92.195	-3.505
38	30.0	60.0	10.0	16.194	-11.554	-92.529	-3.499
39	30.0	68.0	2.0	16.184	-11.519	-93.323	-3.494
40	40.0	10.0	50.0	16.721	-12.503	-92.003	-3.515
41	40.0	20.0	40.0	16.475	-12.036	-91.986	-3.509
42	40.0	30.0	30.0	16.389	-11.865	-92.081	-3.503
43	40.0	40.0	20.0	16.337	-11.757	-92.251	-3.497
44	40.0	50.0	10.0	16.299	-11.677	-92.572	-3.490
45	40.0	58.0	2.0	16.275	-11.625	-93.360	-3.485

TABLE 4b

300°K AND  $1 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	5.4E-03	2.2E-02	3.1E-02	4.4E-02	7.3E-02	6.1E-02	0.
H2	7.1E-05	5.9E-05	6.5E-08	3.7E-02	5.7E-05	9.2E-08	0.
O2	0.	0.	0.	0.	0.	0.	8.3E-02
WATER	9.7E-02	4.3E-02	5.1E-08	4.4E-02	1.1E-02	3.8E-08	4.2E-02
CO	3.0E-10	9.7E-10	1.2E-06	8.0E-18	9.4E-10	6.2E-07	0.
CO2	3.8E-02	6.5E-02	8.8E-02	8.7E-13	1.7E-02	2.3E-02	4.2E-02
BENZENE	0.	3.3E-36	1.2E-08	0.	6.6E-33	2.9E-08	0.
NAPHTHALENE	0.	0.	5.1E-09	0.	0.	1.5E-08	0.
ASPHALT	0.	0.	5.8E-04	0.	0.	2.4E-03	0.
ACETYLENE	0.	2.0E-39	3.0E-30	0.	2.5E-38	4.0E-30	0.
ETHYLENE	1.7E-23	4.0E-22	6.8E-16	4.1E-27	4.8E-21	1.3E-15	0.
ETHANE	4.3E-13	8.6E-12	1.6E-08	5.5E-14	1.0E-10	4.3E-08	0.
FORMIC ACID	6.9E-17	9.9E-17	1.5E-19	8.2E-25	2.5E-17	5.5E-20	0.
ACETIC ACID	2.3E-16	1.6E-15	3.2E-15	4.4E-26	1.4E-15	1.6E-15	0.
FORMALDEHYDE	3.4E-22	9.0E-22	1.3E-21	4.6E-27	8.4E-22	8.9E-22	0.
ACETALDEHYDE	3.6E-25	4.7E-24	8.5E-21	7.8E-32	1.5E-23	8.3E-21	0.
METHANOL	4.6E-20	1.0E-19	1.6E-22	3.3E-22	9.1E-20	1.6E-22	0.
ETHANOL	2.4E-26	2.6E-25	5.2E-25	2.7E-30	8.1E-25	7.3E-25	0.
ACETONE	7.6E-29	4.8E-27	1.1E-20	2.6E-37	5.5E-26	1.5E-20	0.
PROPANE	1.1E-21	1.1E-19	2.7E-13	2.3E-24	4.4E-18	9.9E-13	0.
N2	8.6E-01	8.7E-01	8.8E-01	8.7E-01	9.0E-01	9.1E-01	8.3E-01
NH3	4.0E-07	3.0E-07	1.1E-11	4.7E-03	2.9E-07	1.9E-11	0.
HYDRAZINE	0.	0.	0.	2.0E-37	0.	0.	0.
NO	0.	0.	0.	0.	0.	0.	2.2E-16
NO2	0.	0.	0.	0.	0.	0.	2.3E-12
N2O	0.	0.	0.	0.	0.	0.	5.2E-21
N2O3	0.	0.	0.	0.	0.	0.	1.2E-25
N2O4	0.	0.	0.	0.	0.	0.	2.8E-31
N2O5	0.	0.	0.	0.	0.	0.	3.5E-26
NITROUS ACID	0.	0.	0.	0.	0.	0.	8.6E-17
NITRIC ACID	0.	0.	0.	0.	0.	0.	1.3E-13
NH2OH	3.9E-27	1.6E-27	6.3E-35	4.0E-26	4.1E-28	5.6E-35	0.
NITROMETHANE	0.	0.	0.	0.	0.	0.	0.
HCN	1.5E-23	8.3E-23	3.3E-18	1.1E-26	3.0E-22	3.9E-18	0.
C2N2	0.	0.	1.7E-38	0.	0.	1.6E-38	0.
CYANAMIDE	1.5E-36	7.4E-36	9.7E-33	2.4E-38	2.7E-35	1.4E-32	0.
HNC	1.4E-20	4.1E-20	1.7E-18	8.4E-27	3.9E-20	1.0E-18	0.
METHYL CYANIDE	2.8E-27	7.4E-26	3.8E-18	3.1E-32	9.3E-25	6.2E-18	0.
METH. ISOCYANIDE	3.0E-38	7.9E-37	4.0E-29	0.	9.9E-36	6.5E-29	0.
ETHYL HYDRAZINE	0.	0.	0.	0.	0.	0.	0.
ETHYLENE IMINE	2.5E-38	5.4E-37	3.1E-32	0.	6.5E-36	7.1E-32	0.
METHYL AMINE	8.9E-22	3.3E-21	1.6E-22	1.7E-19	1.1E-20	3.8E-22	0.
DIMETHYL AMINE	6.1E-34	1.1E-32	6.9E-31	1.8E-33	1.3E-31	2.3E-30	0.
TRIMETHYL AMINE	0.	0.	4.2E-37	0.	0.	1.9E-36	0.
ETHENYL AMINE	0.	0.	0.	0.	0.	0.	0.
DIAMINOETHANE	0.	0.	0.	0.	0.	0.	0.
IMIDAZOLE	0.	0.	1.0E-37	0.	0.	1.9E-37	0.
SYMMET. TRIAZINE	0.	0.	0.	0.	0.	0.	0.
NH2SYM. TRIAZINE	0.	0.	0.	0.	0.	0.	0.
ANILINE	0.	0.	1.2E-24	0.	0.	3.3E-24	0.
BENZONITRILE	0.	0.	2.8E-20	0.	0.	5.5E-20	0.
PHEN. ISOCYANIDE	0.	0.	2.9E-31	0.	0.	5.8E-31	0.
QUINOLINE	0.	0.	5.3E-19	0.	0.	1.4E-18	0.
PYRROLE	0.	0.	2.0E-27	0.	0.	4.3E-27	0.
PYRIDINE	0.	0.	1.1E-22	0.	0.	2.3E-22	0.
PYRIMIDINE	0.	0.	6.9E-29	0.	0.	1.3E-28	0.
PURINE	0.	0.	0.	0.	0.	0.	0.
ADENINE	0.	0.	0.	0.	0.	0.	0.
NICOTINIC ACID	0.	0.	1.2E-27	0.	0.	6.5E-28	0.
NICOTINAMIDE	0.	0.	0.	0.	0.	0.	0.
UREA	0.	0.	0.	0.	0.	0.	0.
FORMAMIDE	4.9E-34	1.2E-33	5.5E-35	1.5E-37	1.1E-33	4.8E-35	0.
ACETAMIDE	0.	1.1E-38	6.7E-37	0.	3.6E-38	8.0E-37	0.
METHOXAMINE	1.3E-35	2.6E-35	0.	2.1E-36	2.3E-35	1.7E-39	0.
ETHANOLAMINE	0.	0.	0.	0.	0.	0.	0.
A-ETHYLOLH LAMINE	0.	0.	0.	0.	0.	0.	0.
B-ETHYLOLH LAMINE	0.	0.	0.	0.	0.	0.	0.
OXAMIC ACID	0.	0.	0.	0.	0.	0.	0.
CYANURIC ACID	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
ACETYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
GLYCINE	4.1E-34	2.7E-33	1.7E-34	0.	2.3E-33	1.1E-34	0.
ALANINE	0.	0.	8.1E-39	0.	0.	6.9E-39	0.
PROLINE	0.	0.	0.	0.	0.	0.	0.
SERINE	0.	0.	0.	0.	0.	0.	0.
ASPARTIC ACID	0.	0.	0.	0.	0.	0.	0.
VALINE	0.	0.	0.	0.	0.	0.	0.
LEUCINE	0.	0.	0.	0.	0.	0.	0.
PHENYLALANINE	0.	0.	0.	0.	0.	0.	0.

TABLE 5a

300°K AND 1 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ ,  
 FOR 27 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES  
 OF ALL ELEMENTS. SYSTEMS CONTAINING LIQUID WATER HAVE BEEN OMITTED.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-161.300	-48.153	-0.849	-0.109
2	2.0	9.0	89.0	-161.177	-47.369	-0.907	-0.105
3	2.0	96.0	2.0	-13.588	-2.857	-90.620	-0.080
4	10.0	2.0	88.0	-159.384	-48.072	-0.994	-0.100
5	10.0	10.0	80.0	-159.187	-47.216	-1.088	-0.096
6	10.0	88.0	2.0	-11.090	-3.080	-90.178	-0.065
7	20.0	2.0	78.0	-158.098	-47.919	-1.280	-0.090
8	20.0	10.0	70.0	-157.705	-47.014	-1.472	-0.086
9	20.0	50.0	30.0	2.671	-6.563	-81.927	-0.064
10	20.0	60.0	20.0	3.052	-6.566	-82.315	-0.059
11	20.0	70.0	10.0	3.530	-6.617	-82.894	-0.053
12	22.0	76.0	2.0	15.193	-9.167	-88.726	-0.203
13	18.0	80.0	2.0	-7.249	-3.895	-88.554	-0.051
14	30.0	2.0	68.0	-156.027	-47.497	-2.102	-0.080
15	30.0	10.0	60.0	3.266	-7.203	-81.766	-0.075
16	30.0	20.0	50.0	15.060	-9.803	-87.728	-0.070
17	30.0	30.0	40.0	15.499	-9.821	-88.052	-0.064
18	30.0	40.0	30.0	15.493	-9.752	-88.187	-0.058
19	30.0	50.0	20.0	15.480	-9.694	-88.377	-0.052
20	30.0	60.0	10.0	15.467	-9.645	-88.711	-0.045
21	30.0	68.0	2.0	15.457	-9.611	-89.506	-0.040
22	40.0	10.0	50.0	15.994	-10.595	-88.186	-0.062
23	40.0	20.0	40.0	15.748	-10.128	-88.168	-0.055
24	40.0	30.0	30.0	15.662	-9.956	-88.263	-0.049
25	40.0	40.0	20.0	15.610	-9.848	-88.433	-0.043
26	40.0	50.0	10.0	15.572	-9.768	-88.755	-0.036
27	40.0	58.0	2.0	15.548	-9.717	-89.542	-0.031

TABLE 5b  
 300°K AND 1 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS  
 OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH THREE SELECTED  
 RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80%  
 OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS. SYSTEMS  
 CONTAINING LIQUID WATER HAVE BEEN OMITTED.

COMPOUND	C	E	F
METHANE	7.3E-02	3.1E-02	6.1E-02
H2	1.8E-06	2.9E-09	4.2E-09
O2	0.	0.	0.
WATER	1.1E-02	1.1E-07	7.8E-08
CO	3.0E-11	2.7E-08	1.4E-08
CO2	1.7E-02	8.8E-02	2.3E-02
BENZENE	2.1E-31	1.4E-08	3.4E-08
NAPHTHALENE	0.	1.5E-08	4.5E-08
ASPHALT	0.	5.8E-04	2.4E-03
ACETYLENE	0.	3.2E-32	4.3E-32
ETHYLENE	4.8E-21	3.3E-16	6.2E-16
ETHANE	3.2E-09	3.5E-07	9.5E-07
FORMIC ACID	7.8E-16	6.7E-18	2.5E-18
ACETIC ACID	1.4E-12	3.2E-12	1.6E-12
FORMALDEHYDE	8.4E-22	1.3E-21	8.9E-22
ACETALDEHYDE	4.8E-22	1.9E-19	1.8E-19
METHANOL	2.9E-18	7.1E-21	7.2E-21
ETHANOL	8.1E-22	5.2E-22	7.3E-22
ACETONE	5.5E-23	5.5E-18	7.5E-18
PROPANE	4.4E-15	1.3E-10	4.8E-10
N2	9.0E-01	8.8E-01	9.1E-01
NH3	1.6E-06	1.1E-10	1.9E-10
HYDRAZINE	0.	0.	0.
NO	0.	0.	0.
N2O	0.	0.	0.
N2O3	0.	0.	0.
N2O3	0.	0.	0.
N2O4	0.	0.	0.
N2O5	0.	0.	0.
NITROUS ACID	0.	0.	0.
NITRIC ACID	0.	0.	0.
NH2OH	7.3E-26	2.8E-32	2.5E-32
NITROMETHANE	0.	0.	0.
HCN	5.3E-23	3.4E-19	4.0E-19
C2N2	0.	3.9E-39	3.8E-39
CYANAMIDE	8.4E-34	2.1E-31	3.1E-31
HNC	2.2E-19	8.0E-18	4.9E-18
METHYLCYANAMIDE	5.2E-24	8.6E-18	1.4E-17
METH. ISOCYANIDE	5.5E-35	9.1E-29	1.5E-28
ETHYLHYDRAZINE	0.	0.	0.
ETHYLENEIMINE	1.2E-33	3.2E-30	7.3E-30
METHYLAMINE	2.0E-18	3.4E-20	8.1E-20
DIMETHYLAMINE	7.3E-28	3.3E-27	1.1E-26
TRIMETHYLAMINE	3.7E-35	4.3E-32	2.0E-31
ETHENYLAMINE	0.	1.9E-38	4.4E-38
DIAMINOCETHANE	0.	0.	0.
IMIDAZOLE	0.	2.3E-35	4.5E-35
SYMMET. TRIAZINE	0.	6.4E-37	1.0E-36
NH2SYM. TRIAZINE	0.	0.	0.
ANILINE	0.	3.0E-22	8.6E-22
BENZONITRILE	0.	7.5E-20	1.5E-19
PHEN. ISOCYANIDE	0.	8.0E-31	1.6E-30
QUINOLINE	0.	1.5E-17	4.0E-17
PYRROLE	0.	4.7E-26	1.0E-25
PYRIDINE	0.	1.3E-21	2.7E-21
PYRIMIDINE	0.	7.8E-27	1.4E-26
PURINE	0.	0.	0.
ADELINE	0.	0.	0.
NICOTINIC ACID	0.	1.4E-23	7.6E-24
NICOTINAMIDE	0.	0.	0.
UREA	0.	0.	0.
FORMAMIDE	2.0E-31	1.2E-32	1.0E-32
ACETAMIDE	2.0E-34	3.1E-33	3.7E-33
METHOXYAMINE	1.3E-31	1.3E-35	1.6E-35
ETHANOLAMINE	2.4E-37	6.2E-39	1.1E-38
A-ETHYLOLHOLAMINE	0.	0.	0.
B-ETHYLOLHOLAMINE	0.	0.	0.
OXAMIC ACID	2.3E-38	7.3E-39	1.6E-39
CYANURIC ACID	0.	0.	0.
FORMYLGLYCINE	0.	0.	0.
ACETYLGLYCINE	0.	0.	0.
GLYCINE	4.1E-28	3.7E-29	2.3E-29
ALANINE	1.6E-33	3.8E-32	3.2E-32
PROLINE	0.	0.	0.
SERINE	0.	0.	0.
ASPARTIC ACID	0.	0.	0.
VALINE	0.	1.9E-38	3.0E-38
LEUCINE	0.	0.	0.
PHENYLALANINE	0.	3.1E-37	4.5E-37

TABLE 6a

300°K AND 100 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ ,  
 FOR 13 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER  
 OF MOLES OF ALL ELEMENTS. SYSTEMS CONTAINING LIQUID WATER HAVE BEEN OMITTED.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	22.0	76.0	2.0	14.708	-7.895	-86.181	2.100
2	30.0	20.0	50.0	14.043	-8.397	-84.916	2.233
3	30.0	30.0	40.0	15.014	-8.549	-85.507	2.239
4	30.0	40.0	30.0	15.008	-8.479	-85.642	2.245
5	30.0	50.0	20.0	14.996	-8.422	-85.832	2.251
6	30.0	60.0	10.0	14.983	-8.373	-86.166	2.257
7	30.0	68.0	2.0	14.972	-8.338	-86.961	2.262
8	40.0	10.0	50.0	15.509	-9.322	-85.641	2.241
9	40.0	20.0	40.0	15.263	-8.855	-85.623	2.247
10	40.0	30.0	30.0	15.177	-8.684	-85.718	2.253
11	40.0	40.0	20.0	15.125	-8.576	-85.888	2.260
12	40.0	50.0	10.0	15.087	-8.496	-86.210	2.266
13	40.0	58.0	2.0	15.064	-8.444	-86.997	2.271

TABLE 6b  
 300°K AND 100 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS  
 IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H,  
 O, AND N WITH TWO SELECTED RELATIVE ABUNDANCE RATIOS OF  
 C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF  
 MOLES OF ALL ELEMENTS. SYSTEMS CONTAINING LIQUID  
 WATER HAVE BEEN OMITTED.

COMPOUND	C	F
METHANE	3.1E-02	6.1E-02
H2	3.8E-10	5.3E-10
O2	0.	0.
WATER	1.7E-07	1.3E-07
CO	2.1E-09	1.1E-09
CO2	8.8E-02	2.3E-02
BENZENE	1.6E-08	3.9E-08
NAPHTHALENE	3.1E-08	9.3E-08
ASPHALT	5.8E-04	2.4E-03
ACETYLENE	1.6E-33	2.1E-33
ETHYLENE	2.0E-16	3.8E-16
ETHANE	2.8E-06	7.5E-06
FORMIC ACID	8.6E-17	3.2E-17
ACETIC ACID	3.2E-10	1.6E-10
FORMALDEHYDE	1.3E-21	8.9E-22
ACETALDEHYDE	1.5E-18	1.4E-18
METHANOL	9.0E-20	9.2E-20
ETHANOL	5.2E-20	7.2E-20
ACETONE	3.4E-16	4.6E-16
PROPANE	7.9E-09	2.9E-08
N2	8.8E-01	9.1E-01
NH3	4.9E-10	8.5E-10
HYDRAZINE	0.	0.
NO	0.	0.
NO2	0.	0.
N2O	0.	0.
N2O3	0.	0.
N2O4	0.	0.
N2O5	0.	0.
NITROUS ACID	0.	0.
NITRIC ACID	0.	0.
NH2OH	1.6E-30	1.4E-30
NITROMETHANE	0.	0.
HCN	7.4E-20	8.8E-20
C2N2	1.5E-39	0.
CYANAMIDE	1.7E-30	2.4E-30
HNCO	2.3E-17	1.4E-17
METHYL CYANIDE	1.5E-17	2.4E-17
METH. ISOCYANIDE	1.6E-28	2.6E-28
ETHYL HYDRAZINE	0.	1.5E-39
ETHYLENEIMINE	6.9E-29	1.6E-28
METHYL AMINE	1.2E-18	2.9E-18
DIMETHYL AMINE	9.1E-25	3.0E-24
TRIMETHYL AMINE	9.5E-29	4.3E-28
ETHENYL AMINE	4.2E-37	9.6E-37
DIAMINOTHANE	1.9E-36	7.4E-36
IMIDAZOLE	8.9E-34	1.7E-33
SYMMET. TRIAZINE	6.8E-35	1.1E-34
NH2SYM. TRIAZINE	0.	0.
ANILINE	1.2E-20	3.4E-20
BENZONITRILE	1.5E-19	2.9E-19
PHEN. ISOCYANIDE	1.6E-30	3.1E-30
QUINOLINE	1.4E-16	3.8E-16
PYRROLE	4.0E-25	8.6E-25
PYRIDINE	6.6E-21	1.4E-20
PYRIMIDINE	1.8E-25	3.4E-25
PURINE	0.	0.
ADENINE	0.	0.
NICOTINIC ACID	7.2E-21	3.9E-21
NICOTINAMIDE	0.	0.
UREA	0.	0.
FORMAMIDE	4.2E-31	3.6E-31
ACETAMIDE	8.8E-31	1.0E-30
METHOXAMINE	5.9E-33	7.3E-33
ETHANOLAMINE	2.2E-35	3.8E-35
A-ETHYLOLAMINE	0.	0.
B-ETHYLOLAMINE	4.5E-39	7.6E-39
OXAMIC ACID	2.6E-35	5.8E-36
CYANURIC ACID	0.	0.
FORMYLGLYCINE	0.	0.
ACETYLGLYCINE	0.	0.
GLYCINE	1.3E-25	8.1E-26
ALANINE	1.1E-27	9.1E-28
PROLINE	4.0E-36	4.5E-36
SERINE	0.	0.
ASPARTIC ACID	1.2E-34	2.6E-35
VALINE	3.2E-32	5.2E-32
LEUCINE	1.2E-34	2.6E-34
PHENYLALANINE	7.8E-32	1.1E-31

TABLE 7a

500°K AND  $1 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F_j}{RT}$ ,  
FOR 45 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES  
OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-98.160	-30.419	-4.303	-3.562
2	2.0	9.0	89.0	-98.038	-29.635	-4.361	-3.559
3	2.0	19.0	79.0	-97.832	-29.207	-4.459	-3.554
4	2.0	29.0	69.0	-97.572	-28.928	-4.583	-3.549
5	2.0	39.0	59.0	-97.219	-28.689	-4.754	-3.543
6	2.0	49.0	49.0	-96.670	-28.435	-5.024	-3.538
7	2.0	59.0	39.0	-95.354	-28.011	-5.676	-3.533
8	2.0	69.0	29.0	-93.275	-5.069	-51.731	-3.538
9	2.0	79.0	19.0	-1.582	-4.681	-52.912	-3.544
10	2.0	89.0	9.0	-1.775	-4.469	-54.005	-3.551
11	2.0	96.0	2.0	-2.263	-4.338	-55.765	-3.557
12	10.0	2.0	88.0	-96.245	-30.339	-4.448	-3.554
13	10.0	10.0	80.0	-96.048	-29.483	-4.542	-3.550
14	10.0	20.0	70.0	-95.729	-29.054	-4.696	-3.545
15	10.0	30.0	60.0	-95.259	-28.731	-4.926	-3.540
16	10.0	40.0	50.0	-94.343	-28.356	-5.379	-3.535
17	10.0	50.0	40.0	-2.447	-5.381	-51.328	-3.535
18	10.0	60.0	30.0	-0.018	-4.915	-52.647	-3.537
19	10.0	70.0	20.0	0.576	-4.814	-53.178	-3.535
20	10.0	80.0	10.0	0.803	-4.743	-53.778	-3.532
21	10.0	88.0	2.0	0.550	-4.629	-55.222	-3.533
22	20.0	2.0	78.0	-94.958	-30.185	-4.734	-3.544
23	20.0	10.0	70.0	-94.566	-29.280	-4.926	-3.540
24	20.0	20.0	60.0	-93.650	-28.702	-5.379	-3.535
25	20.0	30.0	50.0	-0.652	-5.435	-51.882	-3.534
26	20.0	40.0	40.0	1.402	-5.143	-52.988	-3.533
27	20.0	50.0	30.0	2.205	-5.137	-53.511	-3.527
28	20.0	60.0	20.0	2.987	-5.212	-54.083	-3.521
29	20.0	70.0	10.0	4.163	-5.417	-54.998	-3.513
30	22.0	76.0	2.0	10.322	-6.572	-58.613	-3.663
31	18.0	80.0	2.0	3.832	-5.302	-55.705	-3.510
32	30.0	2.0	68.0	-92.888	-29.763	-5.556	-3.533
33	30.0	10.0	60.0	2.260	-5.762	-53.144	-3.532
34	30.0	20.0	50.0	5.489	-6.068	-54.846	-3.527
35	30.0	30.0	40.0	8.344	-6.649	-56.439	-3.525
36	30.0	40.0	30.0	10.169	-7.029	-57.629	-3.524
37	30.0	50.0	20.0	10.571	-7.079	-58.124	-3.517
38	30.0	60.0	10.0	10.592	-7.044	-58.591	-3.506
39	30.0	68.0	2.0	10.598	-7.017	-59.826	-3.496
40	40.0	10.0	50.0	10.866	-7.616	-57.759	-3.537
41	40.0	20.0	40.0	10.800	-7.427	-57.844	-3.528
42	40.0	30.0	30.0	10.758	-7.313	-57.986	-3.519
43	40.0	40.0	20.0	10.727	-7.229	-58.216	-3.509
44	40.0	50.0	10.0	10.704	-7.165	-58.658	-3.498
45	40.0	58.0	2.0	10.691	-7.122	-59.890	-3.487

TABLE 7b

500°K AND  $1 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	1.0E-04	1.3E-02	3.2E-02	3.4E-02	6.7E-02	6.2E-02	0.
H2	2.1E-02	3.4E-02	1.7E-03	7.6E-02	2.0E-02	7.6E-04	5.8E-23
O2	0.	0.	0.	0.	0.	0.	8.3E-02
WATER	8.5E-02	2.6E-02	4.1E-05	2.6E-02	2.0E-03	2.1E-06	4.2E-25
CO	8.0E-05	7.1E-04	2.3E-02	1.8E-04	1.5E-03	2.6E-02	4.4E-25
CO2	4.2E-02	7.2E-02	7.5E-02	8.1E-03	2.0E-02	9.6E-03	4.2E-02
BENZENE	2.8E-35	1.2E-24	1.8E-10	3.7E-25	3.8E-18	1.2E-05	0.
NAPHTHALENE	0.	1.5E-39	1.2E-14	0.	1.6E-28	3.0E-06	0.
ASPHALT	0.	0.	6.5E-23	0.	0.	1.7E-03	0.
ACETYLENE	3.6E-25	1.3E-21	6.8E-17	8.7E-22	1.9E-19	2.8E-15	0.
ETHYLENE	1.3E-17	7.3E-14	1.9E-10	1.1E-13	6.1E-12	3.5E-09	0.
ETHANE	2.2E-14	2.0E-10	2.6E-08	6.7E-10	9.7E-09	2.2E-07	0.
FORMIC ACID	2.0E-13	5.4E-13	2.8E-14	1.4E-13	8.8E-14	1.6E-15	5.3E-34
ACETIC ACID	3.9E-17	8.0E-15	2.1E-14	2.4E-15	1.2E-14	5.2E-15	0.
FORMALDEHYDE	8.6E-15	1.2E-13	2.0E-13	6.8E-14	1.5E-13	1.0E-13	0.
ACETALDEHYDE	3.9E-20	4.2E-17	3.5E-15	2.9E-17	4.7E-16	7.5E-15	0.
METHANOL	2.1E-16	4.7E-15	3.8E-16	5.9E-15	3.4E-15	8.6E-17	0.
ETHANOL	1.0E-23	1.8E-20	7.2E-20	2.7E-20	1.2E-19	7.1E-20	0.
ACETONE	3.3E-26	2.7E-21	1.1E-17	2.2E-21	2.8E-19	1.0E-16	0.
PROPANE	3.3E-23	2.3E-17	1.5E-13	9.3E-17	1.0E-14	5.4E-12	0.
N2	8.5E-01	8.5E-01	8.7E-01	8.6E-01	8.9E-01	9.0E-01	8.3E-01
NH3	9.3E-07	1.9E-06	2.1E-08	6.3E-06	8.5E-07	6.5E-09	1.3E-37
HYDRAZINE	1.8E-31	4.8E-31	1.2E-33	2.4E-30	1.7E-31	2.5E-34	0.
NO	2.4E-30	4.6E-31	1.5E-32	2.1E-31	6.3E-32	1.7E-33	4.3E-10
NO2	0.	0.	0.	0.	0.	0.	4.6E-10
N2O	1.5E-35	2.8E-36	9.1E-38	1.3E-36	4.0E-37	1.1E-38	2.6E-15
N2O3	0.	0.	0.	0.	0.	0.	9.8E-21
N2O3	0.	0.	0.	0.	0.	0.	1.6E-25
N2O4	0.	0.	0.	0.	0.	0.	1.5E-25
N2O5	0.	0.	0.	0.	0.	0.	7.3E-31
NITROUS ACID	0.	0.	0.	0.	0.	0.	6.9E-14
NITRIC ACID	0.	0.	0.	0.	0.	0.	1.3E-14
NH2OH	2.5E-20	9.7E-21	3.4E-24	1.5E-20	5.8E-22	1.2E-25	6.3E-31
NITROMETHANE	0.	0.	0.	0.	0.	0.	0.
HGN	1.7E-14	1.0E-12	2.4E-10	8.5E-13	1.3E-11	1.6E-09	0.
C2N2	3.8E-33	8.3E-30	9.1E-24	2.5E-30	2.2E-27	8.4E-22	0.
CYANAMIDE	1.5E-25	1.2E-23	5.9E-22	1.4E-23	1.1E-22	2.7E-21	0.
HNCO	2.0E-14	2.3E-13	1.7E-12	8.6E-14	3.8E-13	1.3E-12	0.
METHYL CYANIDE	2.2E-20	9.9E-17	1.2E-12	1.0E-16	1.1E-14	3.3E-11	0.
METH. ISOCYANIDE	8.1E-27	3.6E-23	4.3E-19	3.6E-23	4.1E-21	1.2E-17	0.
ETHYL CYANIDE	0.	0.	1.5E-39	1.7E-39	6.9E-39	5.9E-39	0.
ETHYLENEIMINE	9.5E-30	6.9E-26	4.0E-23	1.5E-25	4.5E-24	5.1E-22	0.
METHYL AMINE	2.9E-19	4.5E-17	2.5E-17	1.8E-16	1.8E-16	3.4E-17	0.
DIMETHYL AMINE	1.6E-30	1.8E-26	5.2E-25	9.0E-26	6.8E-25	3.0E-24	0.
TRIMETHYL AMINE	0.	9.6E-35	1.4E-31	5.8E-34	3.3E-32	3.5E-30	0.
ETHENYL AMINE	2.1E-35	1.5E-31	8.7E-29	3.3E-31	9.7E-30	1.1E-27	0.
DIAMINOETHANE	0.	6.7E-38	4.3E-37	5.0E-37	2.0E-36	1.7E-36	0.
IMIDAZOLE	0.	6.4E-36	1.8E-29	5.3E-36	8.9E-33	3.2E-27	0.
SYMMET. TRIAZINE	0.	4.1E-38	5.0E-31	2.2E-38	7.5E-35	1.4E-28	0.
NH2SYM. TRIAZINE	0.	0.	0.	0.	0.	0.	0.
ANILINE	0.	1.4E-36	4.4E-23	6.1E-37	3.2E-30	2.0E-18	0.
BENZONITRILE	0.	3.0E-36	2.1E-18	3.4E-37	1.9E-28	2.0E-12	0.
PHEN. ISOCYANIDE	0.	0.	7.6E-25	0.	7.1E-35	7.3E-19	0.
QUINOLINE	0.	0.	5.3E-21	0.	1.4E-33	2.1E-13	0.
PYRROLE	7.0E-39	1.1E-31	7.0E-23	7.6E-32	1.8E-27	7.9E-20	0.
PYRIDINE	0.	4.5E-31	2.9E-19	1.7E-31	1.2E-25	3.1E-15	0.
PYRIMIDINE	0.	4.3E-33	1.2E-23	1.9E-33	9.4E-29	2.1E-20	0.
PURINE	0.	0.	0.	0.	0.	0.	0.
ADENINE	0.	0.	0.	0.	0.	0.	0.
NICOTINIC ACID	0.	1.4E-38	9.1E-27	0.	9.9E-34	1.3E-23	0.
NICOTINAMIDE	0.	0.	0.	0.	0.	2.3E-36	0.
UREA	8.4E-38	2.0E-36	1.6E-37	2.4E-36	1.4E-36	3.7E-38	0.
FORMAMIDE	8.3E-26	1.5E-24	5.4E-25	1.2E-24	1.4E-24	1.9E-25	0.
ACETAMIDE	2.7E-32	3.7E-29	6.8E-28	3.7E-29	3.2E-28	1.0E-27	0.
METHOXAMINE	3.7E-29	1.1E-27	1.9E-29	2.0E-27	6.0E-28	3.0E-30	0.
ETHANOLAMINE	5.7E-38	1.3E-34	1.1E-34	2.8E-34	6.3E-34	7.6E-35	0.
A-ETHYLCHLAMINE	0.	2.8E-38	2.6E-38	6.4E-38	1.4E-37	1.7E-38	0.
B-ETHYLOLHCLAMINE	0.	4.5E-37	4.0E-37	1.0E-36	2.2E-36	2.7E-37	0.
OXAMIC ACID	2.2E-35	6.9E-34	2.6E-34	6.5E-35	1.9E-34	1.1E-35	0.
CYANURIC ACID	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
ACETYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
GLYCINE	4.0E-31	1.0E-28	6.0E-29	4.8E-29	1.2E-28	1.0E-29	0.
ALANINE	0.	1.2E-35	3.5E-34	6.6E-36	1.3E-34	2.6E-34	0.
PROLINE	0.	0.	0.	0.	0.	0.	0.
SERINE	0.	0.	0.	0.	0.	0.	0.
ASPARTIC ACID	0.	0.	0.	0.	0.	0.	0.
VALINE	0.	0.	0.	0.	0.	0.	0.
LEUCINE	0.	0.	0.	0.	0.	0.	0.
PHENYLALANINE	0.	0.	0.	0.	0.	0.	0.

TABLE 8a

500°K AND 1 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ ,  
 FOR 45 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER OF  
 MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-98.160	-28.692	-0.849	-0.109
2	2.0	9.0	89.0	-98.038	-27.908	-0.907	-0.105
3	2.0	19.0	79.0	-97.832	-27.480	-1.005	-0.100
4	2.0	29.0	69.0	-97.572	-27.201	-1.130	-0.095
5	2.0	39.0	59.0	-97.219	-26.962	-1.301	-0.090
6	2.0	49.0	49.0	-96.670	-26.708	-1.570	-0.084
7	2.0	59.0	39.0	-95.354	-26.284	-2.223	-0.079
8	2.0	69.0	29.0	-92.972	-24.431	-49.945	-0.076
9	2.0	79.0	19.0	-7.127	-1.385	-52.470	-0.085
10	2.0	89.0	9.0	-8.339	-1.085	-53.831	-0.094
11	2.0	96.0	2.0	-8.871	-0.954	-55.605	-0.100
12	10.0	2.0	88.0	-96.245	-28.612	-0.994	-0.100
13	10.0	10.0	80.0	-96.048	-27.756	-1.088	-0.096
14	10.0	20.0	70.0	-95.729	-27.327	-1.242	-0.091
15	10.0	30.0	60.0	-95.259	-27.004	-1.472	-0.086
16	10.0	40.0	50.0	-94.343	-26.629	-1.925	-0.081
17	10.0	50.0	40.0	-0.695	-3.130	-48.805	-0.076
18	10.0	60.0	30.0	-0.116	-2.911	-49.358	-0.071
19	10.0	70.0	20.0	-0.305	-2.720	-49.876	-0.066
20	10.0	80.0	10.0	-4.585	-1.610	-52.631	-0.069
21	10.0	88.0	2.0	-6.078	-1.240	-54.993	-0.077
22	20.0	2.0	78.0	-94.958	-28.458	-1.280	-0.090
23	20.0	10.0	70.0	-94.566	-27.553	-1.472	-0.086
24	20.0	20.0	60.0	-93.650	-26.975	-1.925	-0.081
25	20.0	30.0	50.0	0.289	-3.367	-48.920	-0.076
26	20.0	40.0	40.0	1.122	-3.216	-49.441	-0.070
27	20.0	50.0	30.0	1.559	-3.181	-49.797	-0.065
28	20.0	60.0	20.0	1.956	-3.187	-50.191	-0.059
29	20.0	70.0	10.0	2.471	-3.247	-50.784	-0.054
30	22.0	76.0	2.0	9.610	-4.665	-54.375	-0.203
31	18.0	80.0	2.0	-0.913	-2.373	-52.684	-0.052
32	30.0	2.0	68.0	-92.888	-28.037	-2.102	-0.080
33	30.0	10.0	60.0	2.137	-3.820	-49.632	-0.075
34	30.0	20.0	50.0	6.899	-4.657	-52.079	-0.070
35	30.0	30.0	40.0	9.911	-5.317	-53.694	-0.064
36	30.0	40.0	30.0	9.908	-5.248	-53.831	-0.058
37	30.0	50.0	20.0	9.897	-5.191	-54.023	-0.052
38	30.0	60.0	10.0	9.884	-5.142	-54.360	-0.046
39	30.0	68.0	2.0	9.874	-5.108	-55.166	-0.040
40	40.0	10.0	50.0	10.397	-6.069	-53.824	-0.062
41	40.0	20.0	40.0	10.163	-5.621	-53.812	-0.056
42	40.0	30.0	30.0	10.078	-5.452	-53.908	-0.050
43	40.0	40.0	20.0	10.026	-5.345	-54.080	-0.043
44	40.0	50.0	10.0	9.989	-5.266	-54.404	-0.037
45	40.0	58.0	2.0	9.965	-5.214	-55.204	-0.031

TABLE 8b

500°K AND 1 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	4.9E-03	2.1E-02	3.1E-02	4.4E-02	7.3E-02	6.1E-02	0.
H2	1.9E-03	1.6E-03	2.4E-05	4.0E-02	1.5E-03	3.4E-05	1.8E-24
O2	0.	0.	0.	0.	0.	0.	8.3E-02
WATER	9.6E-02	4.3E-02	9.1E-06	4.4E-02	1.0E-02	6.6E-06	4.2E-02
CO	5.8E-06	1.9E-05	1.7E-03	2.6E-09	1.9E-05	8.8E-04	1.4E-26
CO2	3.8E-02	6.6E-02	8.7E-02	3.7E-07	1.7E-02	2.2E-02	4.2E-02
BENZENE	7.5E-28	2.4E-23	6.5E-06	5.0E-34	6.6E-20	1.6E-05	0.
NAPHTHALENE	0.	4.5E-37	3.3E-06	0.	2.5E-31	1.0E-05	0.
ASPHALT	0.	0.	5.3E-04	0.	0.	2.4E-03	0.
ACETYLENE	1.1E-24	3.5E-23	2.2E-17	9.5E-27	4.9E-22	3.0E-17	0.
ETHYLENE	3.5E-15	9.3E-14	9.0E-10	6.3E-16	1.2E-12	1.7E-09	0.
ETHANE	5.4E-10	1.2E-08	1.7E-06	2.0E-09	1.5E-07	4.7E-06	0.
FORMIC ACID	1.6E-11	2.3E-11	4.6E-13	3.2E-15	5.7E-12	1.7E-13	1.7E-32
ACETIC ACID	1.6E-12	1.2E-11	2.4E-11	1.4E-16	1.1E-11	1.2E-11	0.
FORMALDEHYDE	5.6E-14	1.5E-13	2.1E-13	5.2E-16	1.4E-13	1.5E-13	0.
ACETALDEHYDE	1.3E-16	1.9E-15	2.6E-13	5.2E-19	6.4E-15	2.5E-13	0.
METHANOL	1.2E-13	2.8E-13	5.8E-15	2.3E-14	2.5E-13	5.8E-15	0.
ETHANOL	3.1E-18	3.7E-17	7.7E-17	2.6E-19	1.2E-16	1.1E-16	0.
ACETONE	5.8E-20	4.3E-18	5.7E-14	9.8E-23	5.3E-17	7.7E-14	0.
PROPANE	4.2E-16	4.9E-14	6.9E-10	6.8E-16	2.2E-12	2.6E-09	0.
N2	8.6E-01	8.7E-01	8.8E-01	8.7E-01	9.0E-01	9.1E-01	8.3E-01
NH3	2.5E-05	2.0E-05	3.6E-08	2.4E-03	1.8E-05	6.2E-08	7.4E-37
HYDRAZINE	1.5E-27	1.1E-27	2.5E-31	6.7E-25	9.9E-28	5.1E-31	0.
NO	9.6E-31	5.1E-31	7.3E-33	2.1E-32	1.4E-31	3.8E-33	4.3E-10
NO2	0.	0.	0.	0.	0.	0.	1.4E-08
N2O	1.9E-34	1.0E-34	1.4E-36	4.1E-36	2.7E-35	7.7E-37	8.2E-14
NO3	0.	0.	0.	0.	0.	0.	9.8E-18
N2O3	0.	0.	0.	0.	0.	0.	5.1E-21
N2O4	0.	0.	0.	0.	0.	0.	1.5E-19
N2O5	0.	0.	0.	0.	0.	0.	2.3E-23
NITROUS ACID	0.	0.	0.	0.	0.	0.	1.2E-11
NITRIC ACID	0.	0.	0.	0.	0.	0.	7.2E-11
NH2OH	8.5E-18	3.5E-18	9.1E-23	1.8E-17	8.4E-19	8.1E-23	1.1E-28
NITROMETHANE	0.	0.	0.	0.	0.	0.	0.
HCN	3.0E-14	1.7E-13	1.4E-10	2.9E-15	6.5E-13	1.6E-10	0.
C2N2	1.3E-31	4.8E-30	2.1E-22	5.4E-35	7.4E-29	2.1E-22	0.
CYANAMIDE	8.0E-23	4.2E-22	4.1E-20	3.4E-23	1.6E-21	5.9E-20	0.
HNCO	4.4E-13	1.3E-12	1.5E-11	9.0E-16	1.3E-12	9.2E-12	0.
METHYLCYANIDE	2.0E-17	5.9E-16	4.7E-11	8.0E-19	8.1E-15	7.6E-11	0.
METHYLISOCYANIDE	7.3E-24	2.1E-22	1.7E-17	2.9E-25	3.0E-21	2.8E-17	0.
ETHYLYLCYANIDE	3.5E-35	6.8E-34	1.5E-33	2.8E-33	8.1E-33	5.9E-33	0.
ETHYLENEIMINE	7.7E-25	1.9E-23	2.3E-20	6.5E-25	2.5E-22	5.3E-20	0.
METHYLAMINE	4.1E-15	1.7E-14	3.0E-15	1.7E-13	5.6E-14	7.1E-15	0.
DIMETHYLAMINE	1.1E-23	2.4E-22	2.0E-21	2.0E-22	2.9E-21	1.4E-20	0.
TRIMETHYLAMINE	4.2E-31	4.5E-29	7.9E-26	3.1E-30	2.0E-27	3.6E-25	0.
ETHENYLAMINE	1.7E-30	4.2E-29	5.0E-26	1.4E-30	5.4E-28	1.1E-25	0.
DIAMINOETHANE	1.0E-32	1.9E-31	4.3E-31	8.1E-31	2.3E-30	1.7E-30	0.
IMIDAZOLE	3.8E-35	6.3E-33	4.0E-25	1.4E-37	3.0E-31	7.7E-25	0.
SYMMET.-TRIAZINE	1.0E-36	1.8E-34	9.7E-26	0.	1.0E-32	1.6E-25	0.
NH2SYM.-TRIAZINE	0.	0.	2.0E-36	0.	0.	4.0E-36	0.
ANILINE	1.9E-37	5.8E-33	1.9E-16	0.	1.6E-29	5.6E-16	0.
BENZONITRILE	0.	2.1E-34	3.0E-12	0.	2.3E-30	6.1E-12	0.
PHEN.ISCCYANIDE	0.	0.	1.1E-18	0.	8.3E-37	2.2E-18	0.
QUINOLINE	0.	0.	2.5E-12	0.	4.2E-35	6.9E-12	0.
PYRROLE	1.9E-32	1.8E-29	9.2E-19	6.7E-36	3.4E-27	2.0E-18	0.
PYRIDINE	9.3E-33	5.4E-29	1.8E-14	6.7E-38	4.0E-26	3.8E-14	0.
PYRIMIDINE	3.1E-33	3.2E-30	1.3E-18	2.4E-37	6.4E-28	2.5E-18	0.
PURINE	0.	0.	2.4E-39	0.	0.	4.6E-39	0.
ADENINE	0.	0.	0.	0.	0.	0.	0.
NICOTINIC ACID	1.5E-37	1.5E-33	6.6E-19	0.	2.9E-31	3.6E-19	0.
NICOTINAMIDE	0.	0.	1.6E-31	0.	0.	2.0E-31	0.
UREA	5.0E-32	2.0E-31	2.5E-33	9.8E-33	1.1E-31	2.6E-33	0.
FORMAMIDE	1.6E-22	4.1E-22	7.0E-23	6.9E-24	3.8E-22	6.1E-23	0.
ACEITAMIDE	2.7E-26	3.6E-25	6.0E-24	5.0E-28	1.2E-24	7.2E-24	0.
METHOXYSYANIDE	6.5E-24	1.4E-23	3.6E-26	5.8E-24	1.2E-23	4.4E-26	0.
ETHANCLAMINE	5.2E-30	5.7E-29	1.5E-29	2.0E-30	1.8E-28	2.4E-29	0.
A-ETHYLCHLAMINE	1.2E-33	1.3E-32	3.3E-33	4.5E-34	4.1E-32	5.5E-33	0.
B-ETHYLCHLAMINE	1.9E-32	2.0E-31	5.2E-32	7.1E-33	6.5E-31	8.7E-32	0.
OXAMIC ACID	3.9E-29	1.7E-28	3.9E-29	1.6E-35	4.2E-29	8.7E-30	0.
CYANURIC ACID	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	2.2E-38	4.9E-37	0.	1.9E-38	1.5E-37	0.
ACETYLGLYCINE	0.	0.	2.2E-38	0.	0.	9.4E-39	0.
GLYCINE	5.0E-24	3.5E-23	8.4E-24	2.0E-27	3.1E-23	5.1E-24	0.
ALANINE	4.0E-30	1.4E-28	3.4E-27	6.7E-34	4.5E-28	2.8E-27	0.
PROLINE	0.	0.	2.0E-34	0.	0.	2.2E-34	0.
SERINE	6.4E-39	1.2E-37	4.1E-38	0.	1.0E-37	1.8E-38	0.
ASPARTIC ACID	4.9E-39	3.0E-37	9.4E-36	0.	2.5E-37	2.0E-36	0.
VALINE	0.	2.3E-39	5.3E-34	0.	9.8E-38	8.6E-34	0.
LEUCINE	0.	0.	2.1E-37	0.	0.	4.7E-37	0.
PHENYLALANINE	0.	0.	1.7E-31	0.	0.	2.5E-31	0.

TABLE 9a

500°K AND 100 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\bar{F}_i/RT$ ,  
FOR 45 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER OF  
MOLES OF ALL ELEMENTS.

NO.	MCLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-98.160	-27.541	1.454	2.194
2	2.0	9.0	89.0	-98.038	-26.757	1.396	2.198
3	2.0	19.0	79.0	-97.832	-26.329	1.298	2.203
4	2.0	29.0	69.0	-97.572	-26.050	1.173	2.208
5	2.0	39.0	59.0	-97.219	-25.811	1.002	2.213
6	2.0	49.0	49.0	-96.670	-25.557	0.733	2.218
7	2.0	59.0	39.0	-95.354	-25.133	0.080	2.224
8	2.0	69.0	29.0	-4.924	-0.779	-48.633	2.228
9	2.0	79.0	19.0	-8.402	0.094	-50.788	2.225
10	2.0	89.0	9.0	-9.321	0.328	-51.986	2.222
11	2.0	96.0	2.0	-9.729	0.433	-53.687	2.220
12	10.0	2.0	88.0	-96.245	-27.460	1.309	2.202
13	10.0	10.0	80.0	-96.048	-26.604	1.214	2.206
14	10.0	20.0	70.0	-95.729	-26.176	1.060	2.211
15	10.0	30.0	60.0	-95.259	-25.853	0.830	2.217
16	10.0	40.0	50.0	-94.343	-25.477	0.377	2.222
17	10.0	50.0	40.0	-0.669	-1.965	-46.520	2.227
18	10.0	60.0	30.0	-0.130	-1.748	-47.062	2.233
19	10.0	70.0	20.0	-0.389	-1.541	-47.603	2.238
20	10.0	80.0	10.0	-6.075	-0.081	-51.062	2.238
21	10.0	88.0	2.0	-7.197	0.203	-53.226	2.236
22	20.0	2.0	78.0	-94.958	-27.307	1.022	2.212
23	20.0	10.0	70.0	-94.566	-26.402	0.830	2.217
24	20.0	20.0	60.0	-93.650	-25.824	0.377	2.222
25	20.0	30.0	50.0	0.304	-2.205	-46.626	2.227
26	20.0	40.0	40.0	1.112	-2.058	-47.136	2.233
27	20.0	50.0	30.0	1.537	-2.021	-47.487	2.238
28	20.0	60.0	20.0	1.921	-2.025	-47.876	2.244
29	20.0	70.0	10.0	2.405	-2.078	-48.458	2.249
30	22.0	76.0	2.0	9.125	-3.393	-51.820	2.100
31	18.0	80.0	2.0	-3.146	-0.663	-51.493	2.251
32	30.0	2.0	68.0	-92.888	-26.885	0.200	2.223
33	30.0	10.0	60.0	2.128	-2.661	-47.325	2.227
34	30.0	20.0	50.0	8.295	-3.853	-50.473	2.233
35	30.0	30.0	40.0	9.431	-4.046	-51.146	2.239
36	30.0	40.0	30.0	9.425	-3.977	-51.282	2.245
37	30.0	50.0	20.0	9.413	-3.919	-51.472	2.251
38	30.0	60.0	10.0	9.400	-3.870	-51.806	2.257
39	30.0	68.0	2.0	9.390	-3.836	-52.602	2.262
40	40.0	10.0	50.0	9.925	-4.818	-51.280	2.241
41	40.0	20.0	40.0	9.680	-4.353	-51.263	2.247
42	40.0	30.0	30.0	9.595	-4.181	-51.358	2.253
43	40.0	40.0	20.0	9.542	-4.073	-51.528	2.260
44	40.0	50.0	10.0	9.505	-3.994	-51.850	2.266
45	40.0	58.0	2.0	9.481	-3.942	-52.638	2.271

TABLE 9b

500°K AND 100 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	5.3E-03	2.2E-02	3.1E-02	4.5E-02	7.3E-02	6.1E-02	0.
H2	2.0E-04	1.6E-04	3.1E-06	8.5E-03	1.6E-04	4.3E-06	1.8E-25
O2	0.	0.	0.	0.	0.	0.	8.3E-02
WATER	9.7E-02	4.3E-02	1.5E-05	4.5E-02	1.1E-02	1.1E-05	4.2E-02
CO	5.8E-07	1.9E-06	1.4E-04	2.8E-11	1.8E-06	6.9E-05	1.4E-27
CO2	3.8E-02	6.5E-02	8.8E-02	1.9E-08	1.7E-02	2.3E-02	4.2E-02
BENZENE	9.5E-27	2.4E-27	7.4E-06	6.3E-36	4.9E-19	1.8E-05	0.
NAPHTHALENE	0.	4.3E-35	7.1E-06	0.	1.5E-29	2.1E-05	0.
ASPHALT	0.	0.	5.7E-04	0.	0.	2.4E-03	0.
ACETYLENE	1.2E-25	3.5E-24	1.1E-18	1.0E-28	4.4E-23	1.5E-18	0.
ETHYLENE	3.9E-15	9.4E-14	5.6E-10	1.5E-16	1.2E-12	1.1E-09	0.
ETHANE	6.1E-09	1.2E-07	1.4E-05	1.0E-08	1.5E-06	3.7E-05	0.
FORMIC ACID	1.6E-10	2.3E-10	5.9E-12	3.6E-15	5.8E-11	2.2E-12	1.7E-31
ACETIC ACID	1.7E-10	1.2E-09	2.4E-09	7.5E-16	1.1E-09	1.2E-09	0.
FORMALDEHYDE	5.8E-14	1.5E-13	2.1E-13	1.2E-16	1.4E-13	1.5E-13	0.
ACETALDEHYDE	1.4E-15	1.9E-14	2.0E-12	5.8E-19	6.2E-14	2.0E-12	0.
METHANOL	1.3E-12	2.8E-12	7.4E-14	1.1E-13	2.5E-12	7.5E-14	0.
ETHANOL	3.5E-16	3.0E-15	7.7E-15	6.1E-18	1.2E-14	1.1E-14	0.
ACETONE	6.7E-18	4.3E-16	3.5E-12	5.2E-22	4.9E-15	4.8E-12	0.
PROPANE	5.0E-14	5.0E-12	4.3E-08	1.6E-14	2.1E-10	1.6E-07	0.
N2	8.6E-01	8.7E-01	8.8E-01	8.8E-01	9.0E-01	9.1E-01	8.3E-01
NH3	8.3E-05	6.4E-05	1.6E-07	2.4E-02	6.1E-05	2.8E-07	2.4E-36
HYDRAZINE	1.6E-25	1.1E-25	4.0E-29	3.1E-22	1.1E-25	8.3E-29	0.
NO	9.4E-31	5.1E-31	9.3E-33	1.0E-32	1.4E-31	4.9E-33	4.3E-10
NO2	0.	0.	0.	0.	0.	0.	1.4E-07
N2O	1.8E-33	1.0E-33	1.8E-35	2.0E-35	2.8E-34	9.9E-36	8.2E-13
N2O3	0.	0.	0.	0.	0.	0.	9.8E-16
N2O4	0.	0.	0.	0.	0.	0.	5.1E-18
N2O5	0.	0.	0.	0.	0.	0.	1.5E-15
NITROUS ACID	0.	0.	0.	0.	0.	0.	2.3E-18
NITRIC ACID	0.	0.	0.	0.	0.	0.	3.9E-10
NH2OH	2.7E-16	1.1E-16	5.3E-21	8.4E-16	2.9E-17	4.7E-21	3.6E-27
NITROMETHANE	0.	0.	0.	0.	0.	0.	0.
HCN	1.0E-14	5.4E-14	3.1E-11	3.0E-16	2.0E-13	3.6E-11	0.
C2N2	1.3E-31	4.7E-30	8.1E-23	2.7E-36	6.5E-29	7.9E-23	0.
CYANAMIDE	8.4E-22	4.2E-21	3.3E-19	1.7E-22	1.5E-20	4.7E-19	0.
HNCO	1.4E-12	4.2E-12	4.3E-11	4.5E-16	4.1E-12	2.6E-11	0.
METHYL CYANIDE	6.9E-17	1.9E-15	8.1E-11	4.0E-19	2.4E-14	1.3E-10	0.
METH. ISCCYANIDE	2.5E-23	6.8E-22	2.9E-17	1.5E-25	8.6E-21	4.8E-17	0.
ETHYL HYDRAZINE	4.1E-31	7.0E-30	1.5E-29	3.0E-29	8.2E-29	5.9E-29	0.
ETHYLENEDIPIINE	2.8E-23	6.2E-22	5.0E-19	6.9E-24	7.5E-21	1.2E-18	0.
METHYL AMINE	1.4E-13	5.4E-13	1.1E-13	8.0E-12	1.8E-12	2.5E-13	0.
DIMETHYL AMINE	4.2E-21	7.7E-20	1.2E-18	4.5E-20	9.1E-19	3.9E-18	0.
TRIMETHYL AMINE	1.6E-27	1.5E-25	1.7E-22	3.4E-27	6.1E-24	7.8E-22	0.
ETHENYL AMINE	6.0E-29	1.3E-27	1.1E-24	1.5E-29	1.6E-26	2.5E-24	0.
DIAMINODETHANE	1.2E-28	2.0E-27	4.2E-27	8.6E-27	2.4E-26	1.7E-26	0.
IMIDAZOLE	4.3E-33	6.3E-31	1.5E-23	7.4E-37	2.9E-29	2.9E-23	0.
SYMMET. TRIAZINE	3.6E-34	5.8E-32	1.0E-23	9.6E-39	2.8E-30	1.7E-23	0.
NH2SYM. TRIAZINE	0.	0.	7.6E-33	0.	1.5E-38	1.5E-32	0.
ANILINE	7.9E-35	1.8E-30	7.8E-15	0.	3.7E-27	2.3E-14	0.
BENZONITRILE	3.9E-38	6.3E-33	6.0E-12	0.	5.0E-29	1.2E-11	0.
PHEN. ISCCYANIDE	0.	2.3E-39	2.2E-18	0.	1.8E-35	4.3E-18	0.
QUINOLINE	0.	8.3E-38	2.5E-11	0.	8.3E-33	6.5E-11	0.
PYRROLE	7.2E-31	5.6E-28	7.7E-18	3.6E-36	9.1E-26	1.7E-17	0.
PYRIDINE	3.6E-31	1.7E-27	9.4E-14	8.2E-39	9.9E-25	2.0E-13	0.
PYRIMIDINE	3.6E-31	3.1E-28	3.2E-17	2.8E-37	5.3E-26	5.9E-17	0.
PURINE	0.	0.	3.5E-36	0.	0.	6.6E-36	0.
ADENINE	0.	0.	0.	0.	0.	0.	0.
NICOTINIC ACID	5.7E-34	4.6E-30	3.5E-16	0.	7.0E-28	1.9E-16	0.
NICOTINAMIDE	0.	0.	2.3E-28	0.	0.	3.0E-28	0.
UREA	5.3E-29	1.2E-28	3.1E-30	4.8E-30	1.1E-28	3.3E-30	0.
FORMAMIDE	5.4E-21	1.3E-20	2.5E-21	7.4E-23	1.2E-20	2.2E-21	0.
ACETAMIDE	9.6E-24	1.2E-22	1.7E-21	2.6E-26	3.8E-22	2.0E-21	0.
METHOXAMINE	2.2E-21	4.5E-21	1.6E-23	1.3E-21	4.0E-21	2.0E-23	0.
ETHANOLAMINE	1.9E-26	1.9E-25	5.2E-26	2.2E-27	5.9E-25	8.8E-26	0.
A-ETHYLOLAMINE	4.2E-30	4.2E-29	1.2E-29	4.9E-31	1.3E-28	2.0E-29	0.
B-ETHYLCHLAMINE	6.7E-29	6.7E-28	1.8E-28	7.7E-30	2.1E-27	3.1E-28	0.
OXAMIC ACID	1.3E-25	5.5E-25	1.4E-25	9.1E-34	1.3E-25	3.2E-26	0.
CYANURIC ACID	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	3.3E-35	6.9E-34	1.4E-32	0.	5.9E-34	4.3E-33	0.
ACETYLGLYCINE	3.2E-38	3.3E-36	5.0E-33	0.	9.7E-36	2.1E-33	0.
GLYCINE	1.7E-20	1.1E-19	3.0E-20	4.9E-25	9.7E-20	1.8E-20	0.
ALANINE	1.4E-25	4.6E-24	9.4E-23	7.9E-31	1.4E-23	8.0E-23	0.
PROLINE	4.4E-39	4.1E-36	2.7E-29	0.	1.6E-34	3.0E-29	0.
SERINE	2.3E-33	3.9E-32	1.5E-32	0.	3.2E-32	6.5E-33	0.
ASPARTIC ACID	1.8E-32	9.7E-31	2.7E-29	0.	7.6E-31	5.9E-30	0.
VALINE	9.8E-36	7.6E-33	9.3E-28	0.	2.9E-31	1.5E-27	0.
LEUCINE	0.	3.1E-37	2.9E-30	0.	4.1E-35	6.5E-30	0.
PHENYLALANINE	0.	0.	4.4E-26	0.	0.	6.2E-26	0.

TABLE 10a

700°K AND  $1 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F_i}{RT}$ ,  
FOR 45 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES  
OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-71.086	-22.011	-4.303	-3.562
2	2.0	9.0	89.0	-70.964	-21.226	-4.361	-3.559
3	2.0	19.0	79.0	-70.758	-20.799	-4.459	-3.554
4	2.0	29.0	69.0	-70.497	-20.520	-4.583	-3.549
5	2.0	39.0	59.0	-70.145	-20.281	-4.754	-3.543
6	2.0	49.0	49.0	-69.596	-20.027	-5.024	-3.538
7	2.0	59.0	39.0	-68.280	-19.602	-5.676	-3.533
8	2.0	69.0	29.0	-6.839	-5.065	-34.922	-3.538
9	2.0	79.0	19.0	-7.106	-4.604	-36.360	-3.548
10	2.0	89.0	9.0	-4.657	-4.380	-37.790	-3.558
11	2.0	96.0	2.0	0.443	-4.282	-42.128	-3.565
12	10.0	2.0	88.0	-69.171	-21.930	-4.448	-3.554
13	10.0	10.0	80.0	-68.974	-21.074	-4.542	-3.550
14	10.0	20.0	70.0	-68.655	-20.645	-4.696	-3.545
15	10.0	30.0	60.0	-68.185	-20.322	-4.926	-3.540
16	10.0	40.0	50.0	-67.269	-19.947	-5.379	-3.535
17	10.0	50.0	40.0	-9.152	-5.405	-34.450	-3.535
18	10.0	60.0	30.0	-5.464	-4.736	-36.374	-3.545
19	10.0	70.0	20.0	-2.953	-4.494	-37.846	-3.555
20	10.0	80.0	10.0	1.784	-4.378	-41.832	-3.564
21	10.0	88.0	2.0	5.602	-4.524	-47.156	-3.541
22	20.0	2.0	78.0	-67.884	-21.776	-4.734	-3.544
23	20.0	10.0	70.0	-67.492	-20.872	-4.926	-3.540
24	20.0	20.0	60.0	-66.576	-20.293	-5.379	-3.535
25	20.0	30.0	50.0	-7.478	-5.469	-34.949	-3.535
26	20.0	40.0	40.0	-3.647	-4.840	-36.998	-3.545
27	20.0	50.0	30.0	-1.350	-4.632	-38.459	-3.555
28	20.0	60.0	20.0	2.680	-4.528	-42.019	-3.564
29	20.0	70.0	10.0	7.060	-4.830	-46.992	-3.535
30	22.0	76.0	2.0	7.959	-4.620	-48.187	-3.688
31	18.0	80.0	2.0	8.048	-4.977	-49.556	-3.518
32	30.0	2.0	68.0	-65.813	-21.355	-5.556	-3.533
33	30.0	10.0	60.0	-5.486	-5.760	-35.768	-3.535
34	30.0	20.0	50.0	-2.190	-5.125	-37.622	-3.545
35	30.0	30.0	40.0	-0.348	-4.875	-38.897	-3.555
36	30.0	40.0	30.0	3.475	-4.738	-42.395	-3.564
37	30.0	50.0	20.0	8.141	-5.149	-47.386	-3.537
38	30.0	60.0	10.0	8.213	-5.123	-48.115	-3.520
39	30.0	68.0	2.0	8.222	-5.095	-49.705	-3.505
40	40.0	10.0	50.0	0.348	-5.418	-39.217	-3.555
41	40.0	20.0	40.0	4.461	-5.091	-43.080	-3.564
42	40.0	30.0	30.0	8.320	-5.372	-47.173	-3.544
43	40.0	40.0	20.0	8.330	-5.310	-47.554	-3.527
44	40.0	50.0	10.0	8.322	-5.253	-48.204	-3.509
45	40.0	58.0	2.0	8.313	-5.211	-49.774	-3.494

TABLE 10b

700°K AND  $1 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.9E-10	9.1E-07	2.2E-05	1.3E-03	4.3E-02	4.2E-02	0.
H2	2.0E-02	6.2E-02	5.8E-02	1.6E-01	6.4E-02	3.5E-02	1.2E-15
O2	1.2E-27	7.3E-30	1.6E-31	4.6E-34	1.5E-38	1.6E-39	8.3E-02
WATER	8.6E-02	2.1E-02	2.9E-03	4.2E-04	9.7E-07	1.8E-07	4.2E-02
CO	1.1E-03	2.1E-02	8.5E-02	3.8E-02	4.3E-02	4.4E-02	1.3E-16
CO2	4.1E-02	6.2E-02	3.8E-02	9.0E-04	5.8E-06	2.0E-06	4.2E-02
BENZENE	0.	6.7E-35	2.1E-26	1.5E-19	5.7E-07	9.8E-05	0.
NAPHTHALENE	0.	0.	0.	1.5E-30	3.4E-09	3.3E-05	0.
ASPHALT	0.	0.	0.	0.	6.8E-13	2.1E-03	0.
ACETYLENE	2.9E-24	5.4E-19	3.7E-16	7.0E-14	1.1E-09	6.1E-09	0.
ETHYLENE	3.8E-22	2.2E-16	1.4E-13	7.2E-11	4.6E-07	1.4E-06	0.
ETHANE	3.7E-23	6.5E-17	3.9E-14	5.4E-11	1.4E-07	2.4E-07	0.
FORMIC ACID	3.8E-13	1.8E-12	1.0E-12	6.5E-14	1.7E-16	3.2E-17	2.2E-26
ACETIC ACID	4.5E-22	1.6E-18	2.3E-17	3.3E-17	6.9E-18	2.3E-18	0.
FORMALDEHYDE	5.4E-14	3.2E-12	1.2E-11	1.5E-11	6.7E-12	3.8E-12	0.
ACETALDEHYDE	7.1E-24	3.2E-19	3.1E-17	8.4E-16	3.0E-14	3.1E-14	0.
METHANOL	3.4E-18	6.2E-16	2.2E-15	7.1E-15	1.3E-15	4.2E-16	0.
ETHANOL	1.3E-29	1.9E-24	1.7E-22	1.2E-20	1.8E-19	1.0E-19	0.
ACETONE	1.6E-34	5.7E-27	1.4E-23	8.6E-21	2.5E-17	4.4E-17	0.
PROPANE	1.4E-35	1.9E-26	2.8E-22	8.9E-18	1.8E-12	5.5E-12	0.
N2	8.5E-01	8.3E-01	8.2E-01	8.0E-01	8.5E-01	8.8E-01	8.3E-01
NH3	2.5E-08	1.3E-07	1.2E-07	5.2E-07	1.4E-07	5.8E-08	3.4E-28
HYDRAZINE	7.5E-29	7.0E-28	6.0E-28	4.3E-27	7.4E-28	2.4E-28	0.
NO	2.6E-20	2.0E-21	3.0E-22	1.6E-23	9.3E-26	3.1E-26	2.2E-07
NO2	6.2E-35	3.8E-37	8.3E-39	0.	0.	0.	4.3E-09
N2O	8.8E-26	6.7E-27	9.8E-28	5.1E-29	3.1E-31	1.0E-31	7.2E-13
N2O3	0.	0.	0.	0.	0.	0.	1.2E-18
N2O3	0.	0.	0.	0.	0.	0.	4.7E-23
N2O4	0.	0.	0.	0.	0.	0.	3.0E-25
N2O5	0.	0.	0.	0.	0.	0.	1.9E-30
NITROUS ACID	7.2E-32	7.7E-34	1.7E-35	7.6E-38	0.	0.	1.2E-12
NITRIC ACID	0.	0.	0.	0.	0.	0.	4.7E-15
NH2OH	4.5E-18	1.9E-18	2.6E-19	6.0E-20	9.1E-23	1.2E-23	5.2E-25
NITROMETHANE	0.	0.	0.	0.	0.	0.	0.
HCN	1.6E-13	6.8E-11	1.8E-09	2.4E-08	3.1E-06	7.4E-06	0.
C2N2	1.1E-29	6.6E-25	4.7E-22	3.3E-20	1.3E-15	1.4E-14	0.
CYANAMIDE	1.8E-24	1.3E-21	3.2E-20	7.2E-19	6.1E-17	1.1E-16	0.
HNCO	1.5E-13	5.1E-12	2.0E-11	1.4E-11	1.1E-11	8.3E-12	4.4E-33
METHYL CYANIDE	8.2E-24	2.7E-18	1.7E-15	5.4E-13	5.6E-09	2.3E-08	0.
METH-ISOCYANIDE	2.6E-28	8.6E-23	5.6E-20	1.8E-17	1.8E-13	7.6E-13	0.
ETHYL HYDRAZINE	0.	0.	0.	1.0E-37	1.1E-34	1.1E-34	0.
ETHYLENEIMINE	9.6E-34	9.7E-28	5.9E-25	5.0E-22	2.1E-18	4.8E-18	0.
METHYLAMINE	1.7E-23	7.1E-20	1.6E-18	1.6E-16	3.4E-15	2.5E-15	0.
DIMETHYLAMINE	1.2E-37	3.7E-31	2.1E-28	4.8E-25	8.1E-22	1.1E-21	0.
TRIMETHYLAMINE	0.	0.	8.5E-38	4.4E-33	5.9E-28	1.3E-27	0.
ETHENYLAMINE	4.1E-38	4.2E-32	2.5E-29	2.1E-26	8.9E-23	2.1E-22	0.
DIAMINODETHANE	0.	0.	1.5E-39	5.5E-36	6.1E-33	6.0E-33	0.
IMIDAZOLE	0.	7.6E-38	1.3E-33	5.5E-30	7.2E-24	7.3E-23	0.
SYMMET. TRIAZINE	0.	6.7E-39	1.2E-34	3.0E-31	6.3E-25	8.7E-24	0.
NH2SYM. TRIAZINE	0.	0.	0.	0.	1.9E-36	2.0E-35	0.
ANILINE	0.	0.	9.4E-38	1.1E-30	2.7E-18	3.5E-16	0.
BENZONITRILE	0.	0.	1.0E-34	3.8E-27	4.5E-12	3.3E-09	0.
PHEN.ISOCYANIDE	0.	0.	3.4E-39	1.2E-31	1.4E-16	1.1E-13	0.
QUINOLINE	0.	0.	0.	5.1E-34	9.4E-15	3.9E-11	0.
PYRROLE	0.	9.7E-37	4.3E-31	2.6E-26	4.1E-18	9.6E-17	0.
PYRIDINE	0.	1.6E-37	1.9E-30	9.9E-25	3.1E-14	2.3E-12	0.
PYRIMIDINE	0.	5.1E-37	2.3E-31	8.5E-27	2.2E-18	6.9E-17	0.
PURINE	0.	0.	0.	0.	4.5E-39	4.7E-37	0.
ADENINE	0.	0.	0.	0.	0.	0.	0.
NICOTINIC ACID	0.	0.	4.2E-39	5.0E-35	1.0E-26	2.5E-25	0.
NICOTINAMIDE	0.	0.	0.	0.	1.3E-34	7.6E-33	0.
UREA	1.3E-36	2.3E-34	8.1E-34	2.6E-33	5.1E-34	1.7E-34	0.
FORMANICE	2.9E-24	3.0E-22	1.1E-21	2.1E-21	6.3E-22	2.7E-22	0.
ACETAPICINE	2.4E-35	1.9E-30	1.7E-28	7.6E-27	1.0E-25	1.4E-25	0.
METHOXYSYANINE	1.7E-30	5.4E-28	1.8E-27	9.7E-27	1.2E-27	2.8E-28	0.
ETHANOLAMINE	0.	1.5E-37	1.3E-35	1.6E-33	1.5E-32	6.4E-33	0.
A-ETHYLCHLAMINE	0.	1.1E-38	9.0E-37	1.1E-34	1.0E-33	4.4E-34	0.
B-ETHYLCHLAMINE	0.	2.8E-39	2.4E-37	2.9E-35	2.8E-34	1.2E-34	0.
OXAMIC ACID	6.7E-35	1.1E-32	2.3E-32	1.1E-33	2.1E-36	3.0E-37	0.
CYANURIC ACID	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
ACETYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
GLYCINE	3.5E-35	2.2E-31	3.0E-30	7.1E-30	9.7E-31	2.4E-31	0.
ALANINE	0.	0.	1.5E-38	8.4E-37	9.0E-36	4.0E-36	0.
PROLINE	0.	0.	0.	0.	0.	0.	0.
SERINE	0.	0.	0.	0.	0.	0.	0.
ASPARTIC ACID	0.	0.	0.	0.	0.	0.	0.
VALINE	0.	0.	0.	0.	0.	0.	0.
LEUCINE	0.	0.	0.	0.	0.	0.	0.
PHENYLALANINE	0.	0.	0.	0.	0.	0.	0.

TABLE 11a

700°K AND 1 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ ,  
 FOR 45 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER OF  
 MOLES OF ALL ELEMENTS.

NO.	MCLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-71.086	-20.284	-0.849	-0.109
2	2.0	9.0	89.0	-70.964	-19.499	-0.907	-0.105
3	2.0	19.0	79.0	-70.758	-19.072	-1.005	-0.100
4	2.0	29.0	69.0	-70.497	-18.793	-1.130	-0.095
5	2.0	39.0	59.0	-70.145	-18.554	-1.301	-0.090
6	2.0	49.0	49.0	-69.596	-18.300	-1.570	-0.084
7	2.0	59.0	39.0	-68.280	-17.875	-2.223	-0.079
8	2.0	69.0	29.0	-3.132	-1.640	-34.854	-0.083
9	2.0	79.0	19.0	-2.217	-1.274	-35.943	-0.088
10	2.0	89.0	9.0	-2.923	-1.021	-37.159	-0.096
11	2.0	96.0	2.0	-3.461	-0.886	-38.941	-0.103
12	10.0	2.0	88.0	-69.171	-20.203	-0.994	-0.100
13	10.0	10.0	80.0	-68.974	-19.347	-1.088	-0.096
14	10.0	20.0	70.0	-68.655	-18.918	-1.242	-0.091
15	10.0	30.0	60.0	-68.185	-18.596	-1.472	-0.086
16	10.0	40.0	50.0	-67.269	-18.220	-1.925	-0.081
17	10.0	50.0	40.0	-2.380	-1.980	-34.385	-0.080
18	10.0	60.0	30.0	-0.490	-1.577	-35.485	-0.081
19	10.0	70.0	20.0	-0.072	-1.467	-35.979	-0.078
20	10.0	80.0	10.0	-0.045	-1.362	-36.618	-0.076
21	10.0	88.0	2.0	-0.629	-1.181	-38.337	-0.079
22	20.0	2.0	78.0	-67.884	-20.050	-1.280	-0.090
23	20.0	10.0	70.0	-67.492	-19.145	-1.472	-0.086
24	20.0	20.0	60.0	-66.576	-18.567	-1.925	-0.081
25	20.0	30.0	50.0	-0.937	-2.095	-34.766	-0.080
26	20.0	40.0	40.0	0.731	-1.813	-35.703	-0.078
27	20.0	50.0	30.0	1.381	-1.780	-36.167	-0.073
28	20.0	60.0	20.0	1.970	-1.811	-36.665	-0.068
29	20.0	70.0	10.0	2.772	-1.926	-37.442	-0.061
30	22.0	76.0	2.0	7.126	-2.625	-40.560	-0.212
31	18.0	80.0	2.0	2.589	-1.841	-38.371	-0.057
32	30.0	2.0	68.0	-65.813	-19.628	-2.102	-0.080
33	30.0	10.0	60.0	0.896	-2.444	-35.498	-0.079
34	30.0	20.0	50.0	2.776	-2.311	-36.549	-0.077
35	30.0	30.0	40.0	4.042	-2.455	-37.338	-0.074
36	30.0	40.0	30.0	5.392	-2.696	-38.282	-0.072
37	30.0	50.0	20.0	7.248	-3.095	-39.855	-0.070
38	30.0	60.0	10.0	7.401	-3.096	-40.537	-0.056
39	30.0	68.0	2.0	7.420	-3.074	-42.018	-0.043
40	40.0	10.0	50.0	6.695	-3.379	-38.813	-0.092
41	40.0	20.0	40.0	7.508	-3.412	-39.546	-0.088
42	40.0	30.0	30.0	7.537	-3.337	-39.772	-0.076
43	40.0	40.0	20.0	7.531	-3.272	-40.071	-0.063
44	40.0	50.0	10.0	7.521	-3.218	-40.627	-0.048
45	40.0	58.0	2.0	7.514	-3.180	-42.091	-0.034

TABLE 11b

700°K AND 1 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.0E-04	1.3E-02	2.8E-02	3.7E-02	6.5E-02	6.2E-02	0.
H2	1.9E-02	2.7E-02	7.4E-03	6.6E-02	2.1E-02	2.0E-03	3.7E-17
O2	1.4E-30	9.7E-32	3.7E-33	1.6E-32	3.0E-33	6.2E-36	8.3E-02
WATER	8.7E-02	3.2E-02	1.8E-03	3.2E-02	4.5E-03	2.0E-05	4.2E-02
CO	1.0E-03	6.1E-03	3.2E-02	1.1E-03	8.2E-03	3.8E-02	4.1E-18
CO2	4.1E-02	6.6E-02	6.9E-02	4.9E-03	1.6E-02	3.3E-03	4.2E-02
BENZENE	3.8E-27	1.3E-18	1.2E-11	1.9E-19	1.4E-13	1.4E-04	0.
NAPHTHALENE	0.	3.3E-29	4.7E-17	5.3E-31	9.9E-21	1.1E-04	0.
ASPHALT	0.	0.	2.3E-32	0.	0.	1.3E-03	0.
ACETYLENE	2.1E-18	1.4E-15	3.0E-13	7.6E-16	6.9E-14	6.9E-11	0.
ETHYLENE	2.6E-13	2.5E-10	1.5E-08	3.2E-10	9.5E-09	9.3E-07	0.
ETHANE	2.3E-11	3.2E-08	5.1E-07	1.0E-07	9.6E-07	9.1E-06	0.
FORMIC ACID	3.6E-10	8.1E-10	2.3E-10	1.5E-10	1.5E-10	3.1E-12	7.0E-25
ACETIC ACID	3.5E-13	2.5E-11	5.4E-11	5.1E-12	2.9E-11	5.7E-12	0.
FORMALDEHYDE	4.7E-11	4.0E-10	5.9E-10	1.8E-10	4.3E-10	1.9E-10	0.
ACETALDEHYDE	5.1E-15	1.3E-12	1.5E-11	7.0E-13	8.9E-12	3.9E-11	0.
METHANOL	2.8E-12	3.3E-11	1.3E-11	3.7E-11	2.0E-11	1.2E-12	0.
ETHANOL	9.1E-18	3.3E-15	1.0E-14	4.3E-15	1.0E-14	7.5E-15	0.
ACETONE	9.8E-20	8.1E-16	6.9E-14	4.7E-16	3.3E-14	1.4E-12	0.
PROPANE	7.2E-18	3.1E-13	3.8E-11	1.1E-12	5.7E-11	5.3E-09	0.
N2	8.5E-01	8.6E-01	8.6E-01	8.6E-01	8.9E-01	8.9E-01	8.3E-01
NH3	2.2E-05	3.7E-05	5.4E-06	1.4E-04	2.7E-05	8.1E-07	1.9E-27
HYDRAZINE	6.6E-23	1.3E-22	1.0E-23	8.0E-22	8.6E-23	8.0E-25	0.
NO	8.8E-22	2.4E-22	4.6E-23	9.5E-23	4.2E-23	1.9E-24	2.2E-07
N02	2.2E-36	1.6E-37	6.1E-39	2.6E-38	5.0E-39	0.	1.4E-07
N2O	9.4E-26	2.5E-26	4.9E-27	1.0E-26	4.6E-27	2.1E-28	2.3E-11
N03	0.	0.	0.	0.	0.	0.	1.2E-15
N203	0.	0.	0.	0.	0.	0.	1.5E-18
N204	0.	0.	0.	0.	0.	0.	3.0E-19
N205	0.	0.	0.	0.	0.	0.	6.0E-23
NITROUS ACID	8.0E-32	6.8E-33	1.4E-34	1.7E-33	1.9E-34	1.2E-37	2.1E-10
NITRIC ACID	0.	0.	0.	0.	0.	0.	2.6E-11
NH2CH	4.4E-15	2.0E-15	5.6E-17	3.1E-15	2.5E-16	3.4E-19	9.3E-23
NITROMETHANE	0.	0.	0.	0.	0.	0.	0.
HCN	1.3E-10	3.6E-09	5.2E-08	2.6E-09	2.5E-08	8.0E-07	0.
C2N2	8.5E-24	4.3E-21	3.3E-18	9.2E-22	2.6E-19	2.8E-15	0.
CYANAMIDE	1.4E-18	4.5E-17	3.5E-16	5.2E-17	2.9E-16	2.9E-15	0.
HNC	1.4E-10	9.8E-10	2.8E-09	2.9E-10	1.2E-09	1.7E-09	2.5E-32
METHYL CYANIDE	5.7E-15	4.8E-12	5.2E-10	3.9E-12	2.0E-10	6.5E-08	0.
METH. ISOCYANIDE	1.8E-19	1.5E-16	1.7E-14	1.3E-16	6.6E-15	2.1E-12	0.
ETHYL HYDRAZINE	5.7E-33	1.1E-29	4.9E-29	8.7E-29	2.7E-28	2.5E-28	0.
ETHYLENE IMINE	6.3E-22	7.4E-19	2.3E-17	1.5E-18	2.5E-17	7.7E-16	0.
METHYL AMINE	1.3E-14	6.7E-13	7.5E-13	3.0E-12	3.0E-12	8.9E-13	0.
DIMETHYL AMINE	7.4E-23	1.2E-19	1.0E-18	6.0E-19	3.3E-18	9.7E-18	0.
TRIETHYL AMINE	1.3E-30	6.5E-26	4.2E-24	3.7E-25	1.1E-23	3.2E-22	0.
ETHENYL AMINE	2.7E-26	3.2E-23	9.7E-22	6.4E-23	1.1E-21	3.3E-20	0.
DIAMINOETHANE	3.1E-31	5.9E-28	2.6E-27	4.6E-27	1.5E-26	1.3E-26	0.
IMIDAZOLE	3.2E-31	7.1E-27	1.1E-23	4.3E-27	2.1E-24	2.2E-20	0.
SYMMET. TRIAZINE	5.2E-32	9.7E-28	3.0E-24	3.7E-28	3.3E-25	1.1E-20	0.
NH2SYM. TRIAZINE	0.	1.9E-36	3.0E-33	1.1E-36	5.8E-34	5.9E-30	0.
ANILINE	9.8E-36	4.0E-27	1.9E-20	9.0E-28	3.9E-22	1.2E-13	0.
BENZONITRILE	4.4E-36	2.9E-26	1.4E-17	1.2E-27	2.7E-20	9.2E-09	0.
PHEN. ISOCYANIDE	0.	9.3E-31	4.4E-22	3.9E-32	8.6E-25	3.0E-13	0.
QUINOLINE	0.	8.0E-32	7.9E-21	1.0E-33	3.5E-24	1.2E-09	0.
PYRROLE	8.0E-30	4.7E-24	1.1E-19	2.0E-24	9.5E-21	3.0E-15	0.
PYRIDINE	4.7E-30	6.2E-23	3.9E-17	1.2E-23	9.7E-19	3.2E-11	0.
PYRIMIDINE	7.7E-30	3.8E-24	1.7E-19	1.0E-24	8.9E-21	9.1E-15	0.
PURINE	0.	0.	1.7E-38	0.	0.	2.8E-32	0.
ADENINE	0.	0.	0.	0.	0.	0.	0.
NICOTINIC ACID	1.1E-35	2.3E-28	1.5E-22	3.4E-30	8.6E-25	5.9E-18	0.
NICOTINAMIDE	0.	2.5E-38	4.4E-32	0.	4.7E-34	2.2E-26	0.
UREA	1.1E-27	1.3E-26	5.3E-27	1.4E-26	1.1E-26	4.9E-28	0.
FORMAMIDE	2.4E-18	2.4E-17	1.9E-17	1.7E-17	2.4E-17	3.3E-18	0.
ACETAMIDE	1.7E-23	5.2E-21	3.1E-20	4.2E-21	3.1E-20	4.3E-20	0.
METHOXAMINE	1.4E-21	1.9E-20	4.1E-21	3.3E-20	1.5E-20	2.0E-22	0.
ETHANOLAMINE	4.1E-28	1.8E-25	3.0E-25	3.6E-25	8.6E-25	1.1E-25	0.
A-ETHYLCHLAMINE	2.9E-29	1.2E-26	2.0E-26	2.5E-26	6.0E-26	7.9E-27	0.
B-ETHYLCHLAMINE	7.7E-30	3.4E-27	5.5E-27	6.7E-27	1.6E-26	2.1E-27	0.
OXAMIC ACID	5.7E-26	9.2E-25	7.5E-25	4.8E-26	2.1E-25	6.2E-27	0.
CYANURIC ACID	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	1.1E-35	5.7E-33	3.5E-32	3.4E-34	8.2E-33	2.4E-33	0.
ACETYLGLYCINE	0.	1.6E-36	7.4E-35	1.1E-37	1.4E-35	3.9E-35	0.
GLYCINE	2.7E-23	2.2E-21	2.6E-21	7.2E-22	2.3E-21	1.5E-22	0.
ALANINE	5.9E-30	1.5E-26	1.4E-25	5.7E-27	1.0E-25	6.1E-26	0.
PROLINE	0.	2.5E-37	4.5E-34	4.8E-38	7.6E-35	4.7E-32	0.
SERINE	6.0E-37	4.2E-34	7.2E-34	6.2E-35	4.8E-34	1.3E-35	0.
ASPARTIC ACID	1.2E-38	5.1E-35	4.6E-34	1.4E-36	7.8E-35	1.0E-35	0.
VALINE	0.	9.9E-37	5.0E-34	4.7E-37	2.4E-34	1.5E-32	0.
LEUCINE	0.	0.	3.6E-38	0.	1.4E-38	8.5E-36	0.
PHENYLALANINE	0.	0.	5.1E-37	0.	1.5E-39	1.0E-29	0.

TABLE 12a

700°K AND 100 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ ,  
FOR 45 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER OF  
MOLES OF ALL ELEMENTS.

NO.	MCLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-71.086	-19.132	1.454	2.194
2	2.0	9.0	89.0	-70.964	-18.348	1.396	2.198
3	2.0	19.0	79.0	-70.758	-17.920	1.298	2.203
4	2.0	29.0	69.0	-70.497	-17.641	1.173	2.208
5	2.0	39.0	59.0	-70.145	-17.403	1.002	2.213
6	2.0	49.0	49.0	-69.596	-17.149	0.733	2.218
7	2.0	59.0	39.0	-68.280	-16.724	0.080	2.224
8	2.0	69.0	29.0	-62.778	0.057	-33.520	2.226
9	2.0	79.0	19.0	-5.732	0.844	-35.500	2.219
10	2.0	89.0	9.0	-6.877	1.129	-36.823	2.211
11	2.0	96.0	2.0	-7.379	1.254	-38.580	2.206
12	10.0	2.0	88.0	-69.171	-19.052	1.309	2.202
13	10.0	10.0	80.0	-68.974	-18.196	1.214	2.206
14	10.0	20.0	70.0	-68.655	-17.767	1.060	2.211
15	10.0	30.0	60.0	-68.185	-17.444	0.830	2.217
16	10.0	40.0	50.0	-67.269	-17.069	0.377	2.222
17	10.0	50.0	40.0	-1.176	-0.468	-32.719	2.226
18	10.0	60.0	30.0	-0.531	-0.243	-33.294	2.231
19	10.0	70.0	20.0	-0.632	-0.071	-33.788	2.236
20	10.0	80.0	10.0	-3.236	0.629	-35.685	2.234
21	10.0	88.0	2.0	-4.648	0.981	-38.004	2.227
22	20.0	2.0	78.0	-67.884	-18.898	1.022	2.212
23	20.0	10.0	70.0	-67.492	-17.994	0.830	2.217
24	20.0	20.0	60.0	-66.576	-17.415	0.377	2.222
25	20.0	30.0	50.0	-0.179	-0.698	-32.846	2.227
26	20.0	40.0	40.0	0.694	-0.541	-33.388	2.232
27	20.0	50.0	30.0	1.144	-0.506	-33.750	2.237
28	20.0	60.0	20.0	1.556	-0.514	-34.151	2.243
29	20.0	70.0	10.0	2.097	-0.580	-34.758	2.248
30	22.0	76.0	2.0	6.655	-1.352	-37.140	2.098
31	18.0	80.0	2.0	0.132	-0.059	-35.942	2.250
32	30.0	2.0	68.0	-65.813	-18.477	0.200	2.223
33	30.0	10.0	60.0	1.627	-1.140	-33.540	2.227
34	30.0	20.0	50.0	4.103	-1.395	-34.855	2.232
35	30.0	30.0	40.0	6.909	-1.986	-36.397	2.235
36	30.0	40.0	30.0	6.949	-1.931	-36.561	2.241
37	30.0	50.0	20.0	6.948	-1.878	-36.768	2.248
38	30.0	60.0	10.0	6.941	-1.832	-37.128	2.255
39	30.0	68.0	2.0	6.934	-1.799	-38.030	2.262
40	40.0	10.0	50.0	7.383	-2.632	-36.526	2.235
41	40.0	20.0	40.0	7.207	-2.287	-36.544	2.243
42	40.0	30.0	30.0	7.132	-2.133	-36.649	2.249
43	40.0	40.0	20.0	7.084	-2.031	-36.831	2.257
44	40.0	50.0	10.0	7.050	-1.955	-37.178	2.264
45	40.0	58.0	2.0	7.028	-1.906	-38.075	2.270

TABLE 12b

700°K AND 100 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	4.3E-03	2.1E-02	3.2E-02	4.4E-02	7.2E-02	6.1E-02	0.
H2	3.9E-03	3.4E-03	1.9E-04	3.5E-02	3.1E-03	2.6E-04	3.7E-18
O2	3.8E-31	1.0E-31	2.4E-34	1.0E-33	6.4E-33	5.6E-35	8.3E-02
WATER	9.5E-02	4.2E-02	1.1E-04	4.4E-02	9.8E-03	7.5E-05	4.2E-02
CO	1.8E-04	5.9E-04	1.5E-02	1.2E-06	6.1E-04	7.3E-03	4.1E-19
CO2	3.8E-02	6.6E-02	8.0E-02	1.3E-05	1.7E-02	1.9E-02	4.2E-02
BENZENE	4.6E-22	2.2E-17	5.9E-05	1.4E-24	7.9E-14	1.8E-04	0.
NAPHTHALENE	8.3E-35	6.1E-27	5.7E-05	0.	5.5E-21	2.7E-04	0.
ASPHALT	0.	0.	1.6E-04	0.	0.	2.1E-03	0.
ACETYLENE	4.7E-18	1.7E-16	2.4E-12	6.9E-19	2.6E-15	3.5E-12	0.
ETHYLENE	1.2E-11	3.8E-10	2.9E-07	1.6E-11	5.4E-09	5.8E-07	0.
ETHANE	2.3E-08	6.2E-07	2.6E-05	2.7E-07	8.1E-06	7.1E-05	0.
FURMIC ACID	6.9E-09	1.0E-08	6.9E+10	2.1E-11	2.5E-09	2.2E-10	7.0E-24
ACETIC ACID	4.6E-10	3.8E-09	7.1E-09	1.6E-12	3.5E-09	3.3E-09	0.
FORMALDEHYDE	1.7E-10	4.9E-10	6.8E-10	1.0E-11	4.7E-10	4.6E-10	0.
ACETALDEHYDE	1.3E-12	2.1E-11	7.8E-10	8.6E-14	7.4E-11	7.4E-10	0.
METHANOL	2.1E-10	5.2E-10	3.9E-11	1.1E-10	4.6E-10	3.6E-11	0.
ETHANOL	4.7E-14	6.5E-13	1.4E-12	2.8E-14	2.2E-12	1.8E-12	0.
ACETONE	1.7E-15	1.5E-13	1.6E-10	1.3E-16	2.1E-12	2.1E-10	0.
PROPANE	4.8E-13	7.3E-11	8.7E-08	6.4E-12	3.6E-09	3.3E-07	0.
N2	8.6E-01	8.7E-01	8.7E-01	8.7E-01	9.0E-01	9.1E-01	8.3E-01
NH3	2.1E-04	1.7E-04	2.2E-06	5.7E-03	1.5E-04	3.6E-06	6.0E-27
HYDRAZINE	2.8E-20	2.1E-20	6.6E-23	2.3E-18	1.9E-20	1.3E-22	0.
NO	4.7E-22	2.4E-22	1.2E-23	2.4E-23	6.2E-23	5.9E-24	2.2E-07
NO2	6.3E-36	1.7E-36	4.0E-39	1.7E-38	1.1E-37	0.	1.4E-06
N2O	5.0E-25	2.6E-25	1.3E-26	2.6E-26	6.8E-26	6.4E-27	2.3E-10
N3	0.	0.	0.	0.	0.	0.	1.2E-13
N2O3	0.	0.	0.	0.	0.	0.	1.5E-15
N2O4	0.	0.	0.	0.	0.	0.	3.0E-15
N2O5	0.	0.	0.	0.	0.	0.	6.0E-18
NITROUS ACID	1.0E-30	2.5E-31	1.4E-34	8.2E-33	1.6E-32	4.0E-35	6.8E-09
NITRIC ACID	0.	0.	0.	0.	0.	0.	8.3E-09
NH2CH	2.2E-13	9.1E-14	5.9E-17	3.1E-13	2.1E-14	4.6E-17	2.9E-21
NITROMETHANE	4.9E-38	6.8E-38	0.	0.	1.6E-38	0.	0.
HCN	2.0E-10	1.2E-09	1.5E-07	7.9E-11	4.9E-09	1.8E-07	0.
C2N2	9.5E-23	4.1E-21	1.0E-15	1.6E-24	6.9E-20	1.1E-15	0.
CYANAMIDE	1.0E-16	5.7E-16	1.6E-14	1.2E-16	2.2E-15	2.3E-14	0.
HNCO	1.1E-09	3.5E-09	2.0E-08	2.2E-11	3.5E-09	1.2E-08	7.8E-32
METHYL CYANIDE	6.0E-13	2.0E-11	6.7E-08	2.6E-13	3.0E-10	1.2E-07	0.
METH. ISOCYANIDE	1.9E-17	6.5E-16	2.2E-12	8.5E-18	9.8E-15	3.7E-12	0.
ETHYL HYDRAZINE	1.2E-26	2.7E-25	6.6E-25	1.2E-24	3.4E-24	2.5E-24	0.
ETHYLENE IMINE	1.4E-18	4.0E-17	7.3E-15	5.4E-18	5.6E-16	1.7E-14	0.
METHYL AMINE	8.4E-12	3.8E-11	1.4E-11	2.6E-10	1.3E-10	3.2E-11	0.
DIMETHYL AMINE	3.3E-18	8.3E-17	8.4E-16	1.2E-16	1.1E-15	2.7E-15	0.
TRIMETHYL AMINE	3.9E-24	5.5E-22	1.6E-19	1.6E-22	2.7E-20	7.0E-19	0.
ETHENYL AMINE	5.9E-23	1.7E-21	3.1E-19	2.3E-22	2.4E-20	7.4E-19	0.
DIAMINOETHANE	6.2E-25	1.5E-23	3.5E-23	6.6E-23	1.8E-22	1.3E-22	0.
IMIDAZOLE	5.1E-27	1.1E-24	4.1E-19	8.6E-28	6.3E-23	8.7E-19	0.
SYMMET. TRIAZINE	1.8E-27	4.1E-25	6.7E-19	1.0E-28	2.6E-23	1.2E-18	0.
NH2SYM. TRIAZINE	1.3E-34	2.8E-32	1.1E-26	2.3E-35	1.7E-30	2.4E-26	0.
ANILINE	5.3E-29	2.4E-24	1.5E-12	5.0E-31	8.4E-21	5.5E-12	0.
BENZONITRILE	3.9E-30	1.3E-24	7.5E-09	5.1E-34	2.0E-20	2.1E-08	0.
PHEN. ISOCYANIDE	1.2E-34	4.2E-29	2.4E-13	1.7E-38	6.5E-25	6.6E-13	0.
QUINOLINE	3.5E-36	4.3E-29	3.4E-09	0.	1.0E-23	1.4E-08	0.
PYRROLE	1.9E-25	2.3E-22	1.1E-14	1.2E-26	5.4E-20	2.7E-14	0.
PYRIDINE	3.8E-25	3.0E-21	6.9E-11	3.1E-27	2.8E-18	1.8E-10	0.
PYRIMIDINE	4.1E-25	5.4E-22	1.1E-13	8.8E-27	1.3E-19	2.3E-13	0.
PURINE	0.	0.	1.9E-29	0.	2.0E-37	4.6E-29	0.
ADENINE	0.	0.	1.1E-37	0.	0.	3.0E-37	0.
NICOTINIC ACID	8.2E-29	1.1E-24	3.1E-14	2.3E-34	2.7E-22	1.9E-14	0.
NICOTINAMIDE	1.7E-38	4.2E-34	5.6E-23	0.	4.0E-31	8.6E-23	0.
UREA	8.1E-24	2.0E-23	1.6E-24	4.4E-24	1.9E-23	1.5E-24	0.
FORMAMIDE	4.0E-16	1.1E-15	3.5E-16	7.2E-17	1.0E-15	2.8E-16	0.
ACETAMIDE	1.9E-19	2.8E-18	2.6E-17	3.8E-20	1.0E-17	2.9E-17	0.
METHOXYAMINE	4.6E-18	1.1E-15	1.9E-19	7.4E-18	9.3E-18	2.1E-19	0.
ETHANOLAMINE	9.7E-23	1.3E-21	6.3E-22	1.8E-22	4.1E-21	9.7E-22	0.
A-ETHYLCHLAMINE	6.7E-24	8.7E-23	4.4E-23	1.2E-23	2.8E-22	6.7E-23	0.
B-ETHYLCHLAMINE	1.8E-24	2.4E-23	1.2E-23	3.3E-24	7.7E-23	1.8E-23	0.
OXAMIC ACID	8.9E-22	4.0E-21	1.6E-21	5.3E-26	9.9E-22	3.1E-22	0.
CYANURIC ACID	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	1.2E-29	3.1E-28	3.4E-27	8.3E-34	2.9E-28	9.2E-28	0.
ACETYLGLYCINE	7.3E-33	1.0E-30	3.2E-28	5.7E-37	3.6E-30	1.2E-28	0.
GLYCINE	1.6E-18	1.2E-17	5.5E-18	1.7E-20	1.1E-17	3.0E-18	0.
ALANINE	2.4E-23	1.0E-21	1.3E-20	2.9E-25	3.5E-21	9.9E-21	0.
PROLINE	1.3E-34	2.0E-31	3.4E-26	2.2E-37	1.0E-29	3.8E-26	0.
SERINE	1.3E-29	2.9E-28	1.8E-28	8.1E-33	2.5E-28	6.5E-29	0.
ASPARTIC ACID	4.7E-30	3.4E-28	5.2E-27	1.9E-35	3.0E-28	9.4E-28	0.
VALINE	7.5E-33	1.0E-29	9.7E-26	1.2E-34	4.8E-28	1.5E-25	0.
LEUCINE	1.6E-37	1.2E-33	3.2E-28	2.8E-39	2.2E-31	6.8E-28	0.
PHENYLALANINE	0.	1.6E-38	9.5E-24	0.	2.1E-34	1.6E-23	0.

TABLE 13a

1000°K AND  $1 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  
 $\text{J}/\text{RT}$ , FOR 45 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL  
 NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-50.753	-15.649	-4.303	-3.562
2	2.0	9.0	89.0	-50.630	-14.865	-4.361	-3.559
3	2.0	19.0	79.0	-50.424	-14.437	-4.459	-3.554
4	2.0	29.0	69.0	-50.164	-14.158	-4.583	-3.549
5	2.0	39.0	59.0	-49.812	-13.919	-4.755	-3.543
6	2.0	49.0	49.0	-49.262	-13.665	-5.024	-3.538
7	2.0	59.0	39.0	-47.946	-13.240	-5.677	-3.533
8	2.0	69.0	29.0	-15.241	-5.083	-22.150	-3.538
9	2.0	79.0	19.0	-12.938	-4.619	-23.559	-3.548
10	2.0	89.0	9.0	-11.147	-4.390	-24.923	-3.558
11	2.0	96.0	2.0	-0.990	-4.279	-34.880	-3.565
12	10.0	2.0	88.0	-48.838	-15.568	-4.448	-3.554
13	10.0	10.0	80.0	-48.640	-14.712	-4.542	-3.550
14	10.0	20.0	70.0	-48.322	-14.283	-4.696	-3.545
15	10.0	30.0	60.0	-47.852	-13.961	-4.926	-3.540
16	10.0	40.0	50.0	-46.935	-13.585	-5.379	-3.535
17	10.0	50.0	40.0	-14.878	-5.511	-21.470	-3.535
18	10.0	60.0	30.0	-11.782	-4.821	-23.257	-3.545
19	10.0	70.0	20.0	-10.045	-4.544	-24.506	-3.555
20	10.0	80.0	10.0	0.448	-4.370	-34.708	-3.565
21	10.0	88.0	2.0	6.762	-4.350	-42.607	-3.554
22	20.0	2.0	78.0	-47.551	-15.415	-4.734	-3.544
23	20.0	10.0	70.0	-47.159	-14.510	-4.926	-3.540
24	20.0	20.0	60.0	-46.242	-13.932	-5.379	-3.535
25	20.0	30.0	50.0	-14.018	-5.729	-21.559	-3.535
26	20.0	40.0	40.0	-10.966	-5.005	-23.336	-3.545
27	20.0	50.0	30.0	-9.261	-4.705	-24.578	-3.555
28	20.0	60.0	20.0	0.309	-4.514	-33.877	-3.565
29	20.0	70.0	10.0	6.844	-4.476	-41.075	-3.551
30	22.0	76.0	2.0	6.615	-3.894	-41.272	-3.771
31	18.0	80.0	2.0	6.837	-4.418	-42.659	-3.542
32	30.0	2.0	68.0	-45.480	-14.993	-5.557	-3.533
33	30.0	10.0	60.0	-13.435	-6.239	-21.654	-3.535
34	30.0	20.0	50.0	-10.439	-5.333	-23.416	-3.545
35	30.0	30.0	40.0	-8.768	-4.954	-24.648	-3.555
36	30.0	40.0	30.0	0.392	-4.717	-33.555	-3.565
37	30.0	50.0	20.0	6.946	-4.660	-40.484	-3.551
38	30.0	60.0	10.0	6.947	-4.597	-41.148	-3.536
39	30.0	68.0	2.0	6.938	-4.549	-42.723	-3.524
40	40.0	10.0	50.0	-8.398	-5.497	-24.715	-3.555
41	40.0	20.0	40.0	0.454	-5.063	-33.329	-3.565
42	40.0	30.0	30.0	7.110	-4.957	-40.243	-3.552
43	40.0	40.0	20.0	7.090	-4.858	-40.598	-3.536
44	40.0	50.0	10.0	7.062	-4.770	-41.232	-3.521
45	40.0	58.0	2.0	7.040	-4.706	-42.793	-3.508

TABLE 13b

1000°K AND  $1 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	9.0E-15	3.4E-12	3.0E-11	3.9E-06	1.5E-03	1.1E-03	0.
H2	1.6E-02	4.5E-02	5.0E-02	1.6E-01	1.3E-01	1.0E-01	3.9E-10
O2	2.2E-16	5.4E-18	3.9E-19	7.1E-28	2.1E-33	1.8E-33	8.3E-02
WATER	9.0E-02	3.8E-02	1.1E-02	1.6E-06	2.2E-09	1.6E-09	4.2E-02
CO	5.0E-03	3.8E-02	9.3E-02	4.0E-02	4.1E-02	4.2E-02	2.9E-10
CO2	3.8E-02	4.5E-02	2.9E-02	5.4E-07	9.6E-10	9.2E-10	4.2E-02
BENZENE	0.	0.	0.	1.5E-21	3.6E-05	3.2E-05	0.
NAPHTHALENE	0.	0.	0.	8.5E-33	2.2E-05	2.3E-05	0.
ASPHALT	0.	0.	0.	0.	1.6E-03	3.7E-03	0.
ACETYLENE	2.6E-24	1.8E-20	1.6E-18	5.2E-10	1.5E-04	1.5E-04	0.
ETHYLENE	2.1E-26	4.0E-22	4.0E-20	4.2E-11	9.9E-06	7.4E-06	0.
ETHANE	1.0E-30	5.3E-26	5.0E-24	1.9E-14	3.7E-09	2.2E-09	0.
FORMIC ACID	4.5E-13	1.5E-12	1.1E-12	6.3E-17	9.0E-20	6.8E-20	1.2E-20
ACETIC ACID	2.7E-26	1.2E-23	8.7E-23	1.7E-22	1.2E-22	7.6E-23	0.
FORMALDEHYDE	1.1E-13	2.2E-12	6.0E-12	8.3E-12	7.0E-12	5.6E-12	1.5E-28
ACETALDEHYDE	2.1E-27	6.2E-24	1.7E-22	7.4E-18	3.0E-15	2.1E-15	0.
METHANOL	7.7E-20	4.5E-18	1.3E-17	6.0E-17	4.0E-17	2.6E-17	0.
ETHANOL	8.2E-35	6.6E-31	2.0E-29	2.8E-24	9.2E-22	5.1E-22	0.
ACETONE	0.	2.9E-36	7.8E-34	1.1E-24	2.2E-19	1.3E-19	0.
PROPANE	0.	2.2E-39	2.4E-36	2.6E-22	2.4E-14	1.2E-14	0.
N2	8.5E-01	8.3E-01	8.2E-01	8.0E-01	8.2E-01	8.5E-01	8.3E-01
NH3	1.0E-09	4.7E-09	5.5E-09	3.1E-08	2.3E-08	1.6E-08	3.9E-21
HYDRAZINE	4.3E-27	3.2E-26	3.8E-26	3.9E-25	2.6E-25	1.7E-25	0.
NO	1.2E-12	1.0E-13	4.9E-14	2.1E-18	3.6E-21	3.4E-21	2.3E-05
NO2	6.2E-23	1.5E-24	1.1E-25	1.9E-34	0.	0.	2.3E-08
N2O	2.7E-18	4.1E-19	1.1E-19	4.5E-24	8.0E-27	7.6E-27	5.1E-11
NO3	7.2E-39	0.	0.	0.	0.	0.	5.1E-17
N203	0.	0.	0.	0.	0.	0.	3.7E-21
N204	0.	0.	0.	0.	0.	0.	5.9E-25
N205	0.	0.	0.	0.	0.	0.	5.0E-30
NITROUS ACID	1.9E-22	7.6E-24	5.7E-25	1.9E-33	5.0E-39	3.9E-39	1.1E-11
NITRIC ACID	2.2E-33	1.3E-35	2.7E-37	0.	0.	0.	2.4E-15
NH2OH	1.3E-16	9.0E-17	2.8E-17	6.8E-21	8.7E-24	5.7E-24	9.1E-21
NITROMETHANE	0.	1.9E-39	0.	0.	0.	0.	0.
HCN	3.7E-13	3.0E-11	2.8E-10	5.1E-06	2.8E-03	2.8E-03	1.7E-31
C2N2	1.2E-27	2.8E-24	2.2E-22	2.2E-14	8.2E-09	1.0E-08	0.
CYANAMIDE	2.5E-24	3.3E-22	3.3E-21	1.0E-16	5.2E-14	4.6E-14	0.
HNCO	4.1E-13	5.3E-12	1.3E-11	1.0E-11	9.5E-12	8.8E-12	3.7E-24
METHYL CYANAMIDE	3.9E-27	4.4E-23	4.1E-21	2.4E-12	6.3E-07	5.4E-07	0.
METHYL ISCCYANIDE	3.6E-30	4.1E-26	3.8E-24	2.2E-15	5.8E-10	5.0E-10	0.
ETHYL CYCRAZINE	0.	0.	0.	2.2E-39	3.5E-34	1.7E-34	0.
ETHYLENE IMINE	7.6E-38	2.4E-33	2.5E-31	4.6E-22	9.8E-17	6.7E-17	0.
METHYL AMINE	1.9E-27	1.2E-24	1.3E-23	2.5E-18	8.9E-16	5.4E-16	0.
DIMETHYL AMINE	0.	5.4E-39	6.2E-37	3.7E-27	6.4E-22	3.4E-22	0.
TRIMETHYL AMINE	0.	0.	0.	3.0E-36	2.6E-28	1.2E-28	0.
ETHENYL AMINE	0.	0.	1.8E-36	1.9E-34	3.4E-25	7.4E-20	5.0E-20
DIAMINOCETHANE	0.	0.	0.	1.8E-38	2.9E-33	1.4E-33	0.
IMIDAZOLE	0.	0.	0.	1.2E-28	1.8E-20	1.6E-20	0.
SYMMET. TRIAZINE	0.	0.	0.	6.7E-29	1.1E-20	1.1E-20	0.
NH2SYM. TRIAZINE	0.	0.	0.	0.	5.7E-32	5.1E-32	0.
ANILINE	0.	0.	0.	1.5E-32	3.5E-16	2.8E-16	0.
BENZONITRILE	0.	0.	0.	1.5E-26	2.5E-07	2.9E-07	0.
PHEN. ISCCYANIDE	0.	0.	0.	1.4E-29	2.4E-10	2.7E-10	0.
QUINOLINE	0.	0.	0.	6.6E-35	3.2E-10	3.5E-10	0.
PYRROLE	0.	0.	0.	2.3E-26	1.7E-15	1.5E-15	0.
PYRIDINE	0.	0.	0.	8.4E-25	3.9E-11	3.6E-11	0.
PYRIMIDINE	0.	0.	0.	7.3E-26	6.4E-15	6.1E-15	0.
PURINE	0.	0.	0.	0.	1.8E-32	2.0E-32	0.
ADENINE	0.	0.	0.	0.	0.	0.	0.
Nicotinic Acid	0.	0.	0.	6.6E-39	5.4E-28	4.8E-28	0.
Nicotinamide	0.	0.	0.	0.	7.4E-32	6.4E-32	0.
UREA	1.5E-36	8.5E-35	2.5E-34	1.1E-33	7.5E-34	4.9E-34	0.
FORMAMIDE	2.7E-22	9.3E-21	2.6E-20	6.4E-20	4.9E-20	3.5E-20	0.
ACETAMIDE	2.8E-38	1.3E-34	3.8E-33	3.0E-28	1.1E-25	7.0E-26	0.
METHOXAMINE	3.9E-32	3.8E-30	1.2E-29	9.2E-29	5.7E-29	3.2E-29	0.
ETHANCLAMINE	0.	0.	0.	1.2E-36	3.5E-34	1.7E-34	0.
A-ETHYLOLCHLAMINE	0.	0.	0.	5.7E-36	1.7E-33	8.5E-34	0.
B-ETHYLOLCHLAMINE	0.	0.	0.	1.3E-37	4.0E-35	2.0E-35	0.
EXAMIC ACID	4.1E-35	1.7E-33	3.1E-33	1.4E-37	0.	0.	0.
CYANURIC ACID	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
ACETYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
GLYCINE	5.0E-39	3.7E-36	2.8E-35	9.5E-35	6.0E-35	3.5E-35	0.
ALANINE	0.	0.	0.	0.	0.	0.	0.
PROLINE	0.	0.	0.	0.	0.	0.	0.
SERINE	0.	0.	0.	0.	0.	0.	0.
ASPARTIC ACID	0.	0.	0.	0.	0.	0.	0.
VALINE	0.	0.	0.	0.	0.	0.	0.
LEUCINE	0.	0.	0.	0.	0.	0.	0.
PHENYLALANINE	0.	0.	0.	0.	0.	0.	0.

TABLE 14a

1000°K AND 1 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ ,  
FOR 45 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER OF  
MOLES OF ALL ELEMENTS.

NO.	MCLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-50.753	-13.922	-0.849	-0.109
2	2.0	9.0	89.0	-50.630	-13.138	-0.907	-0.105
3	2.0	19.0	79.0	-50.424	-12.710	-1.005	-0.100
4	2.0	29.0	69.0	-50.164	-12.431	-1.130	-0.095
5	2.0	39.0	59.0	-49.812	-12.192	-1.301	-0.090
6	2.0	49.0	49.0	-49.262	-11.938	-1.570	-0.084
7	2.0	59.0	39.0	-47.946	-11.513	-2.223	-0.079
8	2.0	69.0	29.0	-8.334	-1.630	-22.149	-0.084
9	2.0	79.0	19.0	-6.031	-1.166	-23.559	-0.094
10	2.0	89.0	9.0	-4.240	-0.937	-24.923	-0.105
11	2.0	96.0	2.0	-0.968	-0.834	-28.182	-0.110
12	10.0	2.0	88.0	-48.838	-13.841	-0.994	-0.100
13	10.0	10.0	80.0	-48.640	-12.985	-1.088	-0.096
14	10.0	20.0	70.0	-48.322	-12.557	-1.243	-0.091
15	10.0	30.0	60.0	-47.852	-12.234	-1.472	-0.086
16	10.0	40.0	50.0	-46.935	-11.858	-1.925	-0.081
17	10.0	50.0	40.0	-7.970	-2.058	-21.470	-0.081
18	10.0	60.0	30.0	-4.875	-1.367	-23.257	-0.091
19	10.0	70.0	20.0	-3.138	-1.091	-24.506	-0.101
20	10.0	80.0	10.0	0.112	-0.937	-27.544	-0.109
21	10.0	88.0	2.0	3.204	-1.070	-32.117	-0.087
22	20.0	2.0	78.0	-47.551	-13.688	-1.280	-0.090
23	20.0	10.0	70.0	-47.159	-12.783	-1.472	-0.086
24	20.0	20.0	60.0	-46.242	-12.205	-1.925	-0.081
25	20.0	30.0	50.0	-7.110	-2.276	-21.559	-0.081
26	20.0	40.0	40.0	-4.058	-1.551	-23.336	-0.091
27	20.0	50.0	30.0	-2.358	-1.252	-24.575	-0.101
28	20.0	60.0	20.0	0.809	-1.068	-27.517	-0.109
29	20.0	70.0	10.0	4.648	-1.373	-31.940	-0.081
30	22.0	76.0	2.0	5.334	-1.120	-32.925	-0.237
31	18.0	80.0	2.0	5.418	-1.479	-34.287	-0.065
32	30.0	2.0	68.0	-45.480	-13.266	-2.103	-0.080
33	30.0	10.0	60.0	-6.528	-2.786	-21.653	-0.081
34	30.0	20.0	50.0	-3.531	-1.880	-23.416	-0.091
35	30.0	30.0	40.0	-1.860	-1.500	-24.648	-0.101
36	30.0	40.0	30.0	1.474	-1.296	-27.758	-0.109
37	30.0	50.0	20.0	5.526	-1.655	-32.130	-0.084
38	30.0	60.0	10.0	5.609	-1.633	-32.872	-0.066
39	30.0	68.0	2.0	5.621	-1.606	-34.464	-0.052
40	40.0	10.0	50.0	-1.490	-2.043	-24.715	-0.101
41	40.0	20.0	40.0	2.364	-1.648	-28.344	-0.110
42	40.0	30.0	30.0	5.722	-1.886	-31.934	-0.091
43	40.0	40.0	20.0	5.734	-1.825	-32.318	-0.074
44	40.0	50.0	10.0	5.726	-1.768	-32.968	-0.056
45	40.0	58.0	2.0	5.717	-1.726	-34.538	-0.041

TABLE 14b

1000°K AND 1 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	9.0E-09	3.4E-06	3.8E-05	2.6E-03	4.2E-02	3.9E-02	0.
H2	1.6E-02	4.5E-02	5.0E-02	1.5E-01	6.4E-02	3.8E-02	1.2E-11
O2	2.2E-19	5.4E-21	3.9E-22	1.2E-24	1.8E-28	2.8E-29	8.3E-02
WATER	9.0E-02	3.8E-02	1.1E-02	2.0E-03	1.0E-05	2.4E-06	4.2E-02
CO	5.0E-03	3.8E-02	9.3E-02	3.7E-02	4.3E-02	4.4E-02	9.0E-12
CO2	3.8E-02	4.5E-02	2.9E-02	6.4E-04	9.1E-06	3.7E-06	4.2E-02
BENZENE	0.	5.9E-29	4.3E-23	1.7E-16	8.3E-06	5.6E-04	0.
NAPHTHALENE	0.	0.	7.5E-36	2.5E-25	3.9E-07	7.2E-04	0.
ASPHALT	0.	0.	0.	0.	2.5E-11	1.7E-03	0.
ACETYLENE	2.6E-18	1.8E-14	1.6E-12	2.6E-10	9.3E-07	3.8E-06	0.
ETHYLENE	2.1E-17	4.0E-13	4.0E-11	2.0E-08	3.0E-05	7.2E-05	0.
ETHANE	1.0E-18	5.3E-14	5.8E-12	8.8E-09	5.6E-06	8.0E-06	0.
FORMIC ACID	4.5E-10	1.5E-09	1.1E-09	7.2E-11	4.3E-13	1.0E-13	3.8E-19
ACETIC ACID	2.7E-17	1.2E-14	8.7E-14	1.3E-13	3.0E-14	1.1E-14	0.
FORMALDEHYDE	1.1E-10	2.2E-09	6.0E-09	7.4E-09	3.6E-09	2.2E-09	1.5E-28
ACETALDEHYDE	2.1E-18	6.2E-15	1.7E-13	4.5E-12	8.4E-11	8.0E-11	0.
METHANOL	7.7E-14	4.5E-12	1.3E-11	5.1E-11	1.0E-11	3.7E-12	0.
ETHANOL	8.2E-23	6.6E-19	2.0E-17	1.6E-15	1.3E-14	7.3E-15	0.
ACETONE	7.2E-27	2.9E-21	7.7E-19	4.7E-16	3.4E-13	5.1E-13	0.
PROPANE	3.0E-28	2.2E-21	2.4E-18	8.0E-14	2.0E-09	4.4E-09	0.
N2	8.5E-01	8.3E-01	8.2E-01	8.0E-01	8.5E-01	8.8E-01	8.3E-01
NH3	1.0E-06	4.7E-06	5.5E-06	2.9E-05	8.2E-06	3.8E-06	2.2E-20
HYDRAZINE	4.3E-21	3.2E-20	3.8E-20	3.6E-19	6.6E-20	2.4E-20	2.4E-39
NO	3.8E-14	5.8E-15	1.5E-15	8.4E-17	1.1E-18	4.3E-19	2.3E-05
NO2	2.0E-24	4.7E-26	3.3E-27	1.0E-29	1.6E-33	2.5E-34	7.2E-07
N2O	2.7E-18	4.1E-19	1.1E-19	5.9E-21	7.7E-23	3.1E-23	1.6E-09
N2O3	0.	0.	0.	0.	0.	0.	5.1E-14
N2O4	0.	0.	0.	0.	0.	0.	1.2E-16
N2O5	0.	0.	0.	0.	0.	0.	1.6E-22
NITROUS ACID	1.9E-22	7.6E-24	5.7E-25	3.1E-27	3.1E-31	3.7E-32	2.0E-09
NITRIC ACID	2.2E-33	1.3E-35	2.7E-37	0.	0.	0.	1.3E-11
NH2OH	1.3E-13	9.0E-14	2.8E-14	8.3E-15	2.8E-17	5.2E-18	1.6E-18
NITROPENTHANE	3.4E-34	1.8E-33	1.4E-33	1.6E-34	6.5E-37	1.2E-37	0.
HCN	3.7E-10	3.0E-08	2.8E-07	3.6E-06	2.2E-04	4.5E-04	3.0E-32
C2N2	1.2E-21	2.8E-18	2.2E-16	1.1E-14	1.1E-10	7.4E-10	0.
CYANAMIDE	2.5E-18	3.3E-16	3.3E-15	7.1E-14	2.9E-12	4.7E-12	0.
HNCO	4.1E-10	5.3E-09	1.3E-08	9.2E-09	7.0E-09	5.7E-09	2.1E-23
METHYL CYANIDE	3.9E-18	4.4E-14	4.1E-12	1.1E-09	2.7E-06	8.7E-06	0.
METH. ISCCYANIDE	3.6E-21	4.1E-17	3.8E-15	1.1E-12	2.5E-09	8.1E-09	0.
ETHYL HYDRAZINE	1.2E-38	1.7E-33	2.1E-31	9.5E-28	2.7E-25	2.3E-25	0.
ETHYLENE IMINE	7.6E-26	2.4E-21	2.5E-19	2.1E-16	2.1E-13	4.0E-13	0.
METHYL AMINE	1.9E-18	1.2E-15	1.3E-14	1.6E-12	1.7E-11	1.3E-11	0.
DIMETHYL AMINE	6.3E-29	5.4E-24	6.2E-22	1.6E-18	6.9E-16	7.8E-16	0.
TRIMETHYL AMINE	0.	1.4E-32	1.6E-29	9.3E-25	1.5E-20	2.7E-20	0.
ETHENYL AMINE	5.7E-29	1.8E-24	1.9E-22	1.6E-19	1.6E-16	3.0E-16	0.
DIAMINOETHANE	1.0E-37	1.5E-32	1.7E-30	8.0E-27	2.3E-24	2.0E-24	0.
IMIDAZOLE	1.5E-35	1.4E-29	1.2E-26	4.2E-23	6.3E-18	4.1E-17	0.
SYMMET. TRIAZINE	2.6E-35	1.4E-29	1.2E-26	2.3E-23	5.5E-18	4.7E-17	0.
NH2SYM. TRIAZINE	0.	4.4E-38	3.8E-35	1.3E-31	2.1E-26	1.4E-25	0.
ANILINE	0.	3.3E-37	2.5E-31	1.8E-24	5.7E-14	3.0E-12	0.
BENZONITRILE	0.	1.3E-35	8.0E-29	1.3E-21	9.4E-09	2.2E-06	0.
PHEN. ISCCYANIDE	0.	1.2E-38	7.4E-32	1.2E-24	8.7E-12	2.0E-09	0.
QUINOLINE	0.	0.	1.1E-36	2.8E-27	7.3E-11	6.9E-08	0.
PYRROLE	1.8E-37	1.4E-29	1.2E-25	5.3E-21	4.7E-14	6.1E-13	0.
PYRIDINE	1.5E-39	5.9E-30	4.5E-25	1.4E-19	1.2E-10	4.0E-09	0.
PYRIMIDINE	1.9E-36	8.9E-29	7.1E-25	1.8E-20	2.5E-13	4.2E-12	0.
PURINE	0.	0.	0.	6.0E-38	8.2E-29	3.8E-27	0.
ADENINE	0.	0.	0.	0.	1.0E-37	3.7E-36	0.
NICOTINIC ACID	0.	3.9E-36	1.9E-31	1.3E-27	1.6E-20	2.1E-19	0.
NICOTINAMIDE	0.	0.	0.	2.6E-34	1.6E-25	4.5E-24	0.
UREA	1.5E-27	8.5E-26	2.5E-25	9.3E-25	2.0E-25	7.4E-26	0.
FORMAMIDE	2.7E-16	9.3E-15	2.6E-14	5.6E-14	1.8E-14	8.5E-15	1.0E-38
ACETAMIDE	2.8E-26	1.3E-22	3.8E-21	1.8E-19	2.2E-18	1.7E-18	0.
METHOXYAMINE	3.9E-23	3.8E-21	1.2E-20	7.7E-20	1.0E-20	2.9E-21	0.
ETHANCLAMINE	1.1E-32	1.5E-28	4.5E-27	6.6E-25	3.5E-24	1.5E-24	0.
A-ETHYLOLHOLAMINE	5.5E-32	7.3E-28	2.2E-26	3.3E-24	1.7E-23	7.6E-24	0.
B-ETHYLOLHOLAMINE	1.3E-33	1.7E-29	5.2E-28	7.6E-26	4.0E-25	1.8E-25	0.
OXAMIC ACID	4.1E-26	1.7E-24	3.1E-24	1.5E-25	6.7E-28	1.3E-28	0.
CYANURIC ACID	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	1.3E-37	7.7E-34	1.4E-32	1.5E-32	2.6E-33	7.8E-34	0.
ACETYLGLYCINE	0.	0.	5.8E-38	1.3E-36	9.3E-36	4.3E-36	0.
GLYCINE	5.0E-27	3.7E-24	2.8E-23	7.3E-23	1.1E-23	3.3E-24	0.
ALANINE	8.5E-37	8.8E-32	6.6E-30	3.8E-28	2.3E-27	1.0E-27	0.
PROLINE	0.	0.	0.	1.8E-37	3.8E-33	7.1E-33	0.
SERINE	0.	2.6E-37	5.2E-36	1.7E-35	1.2E-36	2.2E-37	0.
ASPARTIC ACID	0.	0.	1.4E-38	1.8E-38	1.5E-39	0.	0.
VALINE	0.	0.	0.	1.6E-38	1.5E-34	1.6E-34	0.
LEUCINE	0.	0.	0.	0.	5.1E-38	8.6E-38	0.
PHENYLALANINE	0.	0.	0.	0.	5.5E-33	2.8E-31	0.

TABLE 15a

1000°K AND 100 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ ,  
 FOR 45 SYSTEMS OF C, H, O, AND N. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES  
 OF ALL ELEMENTS.

NO.	MCLE PERCENTAGE			FREE ENERGIES (F/MOLE)			
	C	H	O	C	H	O	N
1	2.0	2.0	96.0	-50.753	-12.771	1.454	2.194
2	2.0	9.0	89.0	-50.630	-11.986	1.396	2.198
3	2.0	19.0	79.0	-50.424	-11.559	1.298	2.203
4	2.0	29.0	69.0	-50.164	-11.280	1.173	2.208
5	2.0	39.0	59.0	-49.811	-11.041	1.002	2.213
6	2.0	49.0	49.0	-49.262	-10.787	0.733	2.218
7	2.0	59.0	39.0	-47.946	-10.362	0.080	2.224
8	2.0	69.0	29.0	-3.844	0.653	-22.104	2.219
9	2.0	79.0	19.0	-2.641	1.045	-23.271	2.213
10	2.0	89.0	9.0	-3.035	1.276	-24.434	2.206
11	2.0	96.0	2.0	-3.511	1.406	-26.198	2.200
12	10.0	2.0	88.0	-48.838	-12.690	1.309	2.202
13	10.0	10.0	80.0	-48.640	-11.834	1.214	2.206
14	10.0	20.0	70.0	-48.322	-11.405	1.060	2.211
15	10.0	30.0	60.0	-47.852	-11.082	0.830	2.217
16	10.0	40.0	50.0	-46.935	-10.707	0.377	2.222
17	10.0	50.0	40.0	-3.379	0.241	-21.462	2.222
18	10.0	60.0	30.0	-1.162	0.762	-22.799	2.218
19	10.0	70.0	20.0	-0.640	0.900	-23.389	2.220
20	10.0	80.0	10.0	-0.492	1.001	-24.100	2.223
21	10.0	88.0	2.0	-0.755	1.126	-25.732	2.223
22	20.0	2.0	78.0	-47.551	-12.536	1.022	2.212
23	20.0	10.0	70.0	-47.159	-11.632	0.830	2.217
24	20.0	20.0	60.0	-46.242	-11.053	0.377	2.222
25	20.0	30.0	50.0	-2.543	0.017	-21.539	2.222
26	20.0	40.0	40.0	-0.264	0.548	-22.872	2.218
27	20.0	50.0	30.0	0.420	0.649	-23.417	2.221
28	20.0	60.0	20.0	0.940	0.668	-23.962	2.226
29	20.0	70.0	10.0	1.626	0.605	-24.856	2.234
30	22.0	76.0	2.0	4.655	0.263	-27.635	2.087
31	18.0	80.0	2.0	2.030	0.568	-26.510	2.243
32	30.0	2.0	68.0	-45.480	-12.115	0.200	2.223
33	30.0	10.0	60.0	-1.924	-0.484	-21.653	2.222
34	30.0	20.0	50.0	0.597	0.234	-23.127	2.216
35	30.0	30.0	40.0	1.467	0.336	-23.767	2.217
36	30.0	40.0	30.0	2.295	0.290	-24.480	2.221
37	30.0	50.0	20.0	4.011	-0.027	-26.132	2.228
38	30.0	60.0	10.0	5.012	-0.235	-27.685	2.244
39	30.0	68.0	2.0	5.047	-0.219	-29.271	2.259
40	40.0	10.0	50.0	2.704	-0.218	-24.408	2.207
41	40.0	20.0	40.0	3.975	-0.274	-25.536	2.208
42	40.0	30.0	30.0	5.126	-0.462	-26.792	2.219
43	40.0	40.0	20.0	5.158	-0.416	-27.174	2.235
44	40.0	50.0	10.0	5.160	-0.370	-27.811	2.253
45	40.0	58.0	2.0	5.156	-0.335	-29.361	2.268

TABLE 15b

1000°K AND 100 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, D, AND N WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N CONSTITUTES 80% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	8.8E-05	6.8E-03	1.6E-02	3.3E-02	5.6E-02	5.8E-02	0.
H2	1.6E-02	3.0E-02	2.0E-02	7.4E-02	3.4E-02	6.3E-03	1.2E-12
O2	2.3E-21	1.4E-22	2.3E-23	1.2E-23	2.6E-24	9.0E-27	8.3E-02
WATER	9.0E-02	4.1E-02	1.1E-02	2.9E-02	6.3E-03	6.9E-05	4.2E-02
CO	4.9E-03	2.7E-02	6.3E-02	6.3E-03	2.5E-02	4.3E-02	9.0E-13
CO2	3.8E-02	5.1E-02	4.8E-02	3.5E-03	6.3E-03	6.5E-04	4.2E-02
BENZENE	1.6E-24	1.3E-15	1.2E-11	5.2E-15	1.6E-10	6.8E-04	0.
NAPHTHALENE	2.2E-38	8.4E-24	5.1E-17	3.2E-23	2.2E-15	1.3E-03	0.
ASPHALT	0.	0.	8.1E-35	0.	6.8E-32	6.5E-04	0.
ACETYLENE	2.5E-14	2.3E-11	4.9E-10	3.7E-11	1.2E-09	1.9E-07	0.
ETHYLENE	2.0E-11	3.5E-08	4.8E-07	1.4E-07	1.9E-06	5.9E-05	0.
ETHANE	9.6E-11	3.1E-07	2.7E-06	2.9E-06	1.9E-05	1.1E-04	0.
FORMIC ACID	4.4E-08	1.1E-07	6.8E-08	1.9E-08	1.5E-08	3.0E-10	3.8E-18
ACETIC ACID	2.6E-11	2.7E-09	6.1E-09	8.9E-10	2.8E-09	2.9E-10	0.
FORMALDEHYDE	1.0E-08	1.1E-07	1.6E-07	6.1E-08	1.1E-07	3.5E-08	1.5E-28
ACETALDEHYDE	2.0E-12	8.6E-10	4.8E-09	9.8E-10	6.5E-09	1.2E-08	0.
METHANOL	7.5E-10	1.4E-08	1.4E-08	2.0E-08	1.6E-08	9.8E-10	0.
ETHANOL	7.8E-15	6.1E-12	2.2E-11	1.7E-11	5.2E-11	1.7E-11	0.
ACETONE	6.8E-17	1.2E-12	2.5E-11	2.7E-12	6.7E-11	6.6E-10	0.
PROPANE	2.8E-16	3.7E-11	1.2E-09	7.1E-10	1.7E-08	5.3E-07	0.
N2	8.5E-01	8.4E-01	8.4E-01	8.5E-01	8.7E-01	8.9E-01	8.3E-01
NH3	1.0E-04	2.6E-04	1.4E-04	1.0E-03	3.1E-04	2.5E-05	6.9E-20
HYDRAZINE	4.2E-17	1.4E-16	6.1E-17	8.8E-16	1.9E-16	6.6E-18	2.4E-37
N0	3.8E-15	9.2E-16	3.8E-16	2.7E-16	1.3E-16	7.7E-18	2.3E-05
N02	2.0E-25	1.2E-26	2.0E-27	1.0E-27	2.3E-28	8.0E-31	7.2E-06
N2O	2.7E-18	6.6E-19	2.7E-19	1.9E-19	9.4E-20	5.6E-21	1.6E-08
N03	0.	0.	0.	0.	0.	0.	5.1E-12
N203	0.	0.	0.	0.	0.	0.	1.2E-13
N204	0.	0.	0.	0.	0.	0.	5.9E-15
N205	0.	0.	0.	0.	0.	0.	1.6E-17
NITROUS ACID	2.0E-22	1.6E-23	2.1E-24	2.1E-24	3.2E-25	4.9E-28	6.2E-08
NITRIC ACID	2.2E-33	4.4E-35	2.4E-36	1.7E-36	1.2E-37	0.	4.2E-09
NH2OH	1.3E-11	7.8E-12	1.7E-12	9.0E-12	1.3E-12	6.2E-15	5.1E-17
NITROMETHANE	3.4E-30	1.1E-29	5.7E-30	3.0E-30	1.7E-30	1.4E-32	0.
HCN	3.6E-08	1.1E-06	5.0E-06	1.4E-06	7.9E-06	1.0E-04	9.5E-33
C2N2	1.1E-17	5.7E-15	1.8E-13	3.6E-15	2.6E-13	2.3E-10	0.
CYANAMIDE	2.4E-14	1.0E-12	3.7E-12	2.0E-12	7.7E-12	4.3E-11	0.
HNCO	4.1E-08	3.1E-07	5.7E-07	1.1E-07	3.0E-07	2.3E-07	6.5E-23
METHYLCYANIDE	3.7E-12	4.7E-09	7.9E-08	1.2E-08	2.5E-07	1.8E-05	0.
METHYLISCCYANIDE	3.4E-15	4.4E-12	7.4E-11	1.1E-11	2.3E-10	1.6E-08	0.
ETHYLHYDRAZINE	1.2E-26	6.8E-23	3.9E-22	1.6E-21	4.9E-21	5.2E-21	0.
ETHYLENEIMINE	7.3E-18	1.7E-14	1.9E-13	1.0E-13	1.0E-12	1.3E-11	0.
METHYLAMINE	1.8E-12	1.9E-10	3.7E-10	1.4E-09	1.7E-09	7.5E-10	0.
DIMETHYLAMINE	6.0E-19	2.6E-15	1.9E-14	3.9E-14	1.7E-13	4.2E-13	0.
TRIMETHYLAMINE	1.1E-25	2.0E-20	5.2E-19	5.8E-19	9.6E-18	1.3E-16	0.
ETHENYLAMINE	5.5E-21	1.3E-17	1.4E-16	7.9E-17	7.6E-16	1.0E-14	0.
DIAMIACETHANE	9.7E-26	5.7E-22	3.3E-21	1.4E-20	4.1E-20	4.4E-20	0.
IMIDAZOLE	1.4E-25	5.4E-21	4.2E-19	1.7E-20	2.0E-18	1.9E-15	0.
SYMMET. TRIAZINE	2.4E-25	6.9E-21	6.6E-19	1.4E-20	2.5E-18	5.3E-15	0.
NH2SYM-TRIAZINE	4.6E-32	1.8E-27	1.4E-25	5.6E-27	6.9E-25	6.4E-22	0.
ANILINE	5.6E-31	6.2E-22	4.6E-18	3.8E-21	8.0E-17	1.5E-10	0.
BENZONITRILE	1.2E-30	1.6E-20	1.0E-15	3.2E-20	1.2E-14	3.6E-06	0.
PHEN.ISCCYANIDE	1.1E-33	1.5E-23	9.5E-19	3.0E-23	1.1E-17	3.4E-09	0.
QUINOLINE	2.5E-38	3.2E-25	4.2E-19	9.8E-25	1.2E-17	5.7E-07	0.
PYRROLE	1.7E-25	2.0E-19	7.1E-17	7.9E-19	5.3E-16	6.1E-12	0.
PYRIDINE	1.4E-25	3.7E-18	7.4E-15	1.2E-17	6.4E-14	2.2E-08	0.
PYRIMIDINE	1.8E-24	1.6E-18	6.8E-16	3.9E-18	3.9E-15	1.1E-10	0.
PURINE	0.	3.8E-34	9.3E-31	7.6E-34	6.5E-30	5.3E-24	0.
ADENINE	0.	0.	6.3E-38	0.	5.9E-37	2.1E-31	0.
NICOTINIC ACID	7.6E-30	2.7E-22	5.1E-19	5.8E-23	5.9E-19	2.1E-14	0.
NICOTINAMIDE	1.1E-37	2.3E-29	8.4E-26	2.6E-29	3.8E-25	9.9E-20	0.
UREA	1.5E-21	2.7E-20	2.7E-20	3.9E-20	3.2E-20	2.0E-21	0.
FORMAMIDE	2.6E-12	3.6E-11	4.4E-11	3.3E-11	3.9E-11	5.6E-12	3.2E-37
ACETAMIDE	2.7E-18	1.5E-15	6.9E-15	2.8E-15	1.3E-14	9.8E-15	0.
METHOXYAMINE	3.8E-17	9.7E-16	7.7E-16	2.2E-15	1.2E-15	3.1E-17	0.
ETHANOLAMINE	1.1E-22	1.1E-19	3.3E-19	5.0E-19	1.0E-18	1.5E-19	0.
A-ETHYLCHLAMINE	5.2E-22	5.5E-19	1.6E-18	2.5E-18	5.1E-18	7.4E-19	0.
B-ETHYLCHLAMINE	1.2E-23	1.3E-20	3.8E-20	5.7E-20	1.2E-19	1.7E-20	0.
OXAMIC ACID	4.0E-20	7.5E-19	8.5E-19	4.6E-20	1.0E-19	1.5E-21	0.
CYANURIC ACID	6.2E-38	2.6E-35	1.6E-34	1.3E-36	2.4E-35	1.1E-35	0.
FORMYLGLYCINE	1.3E-27	9.9E-25	4.2E-24	1.2E-25	1.0E-24	8.1E-26	0.
ACETYLGLYCINE	3.8E-32	1.2E-27	1.9E-26	3.0E-28	9.3E-27	4.1E-27	0.
GLYCINE	4.8E-19	6.8E-17	1.2E-16	3.6E-17	7.6E-17	3.5E-18	0.
ALANINE	8.1E-25	4.7E-21	3.2E-20	4.9E-21	3.9E-20	1.0E-20	0.
PROLINE	3.7E-36	2.0E-29	2.8E-27	3.2E-29	8.1E-27	3.4E-25	0.
SERINE	1.5E-29	2.2E-26	6.1E-26	6.6E-27	2.5E-26	3.8E-28	0.
ASPARTIC ACID	2.2E-31	1.7E-27	1.1E-26	1.2E-28	1.8E-27	4.7E-29	0.
VALINE	3.5E-36	3.5E-29	3.3E-27	1.4E-28	1.6E-26	1.2E-25	0.
LEUCINE	0.	4.2E-33	1.4E-30	3.3E-32	1.4E-29	6.1E-28	0.
PHENYLALANINE	0.	3.9E-36	3.6E-31	6.3E-36	3.4E-30	2.0E-23	0.

TABLE 16a

300°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND CL. N, P, S, AND CL CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	CL	S
1	2.0	2.0	96.0	-161.299	-49.874	-4.291	-8.848	-280.697	-8.859	-168.632
2	2.0	9.0	89.0	-161.177	-49.082	-4.334	-8.830	-280.581	-8.855	-168.467
3	2.0	19.0	79.0	-160.970	-48.643	-4.409	-8.802	-280.378	-8.842	-168.185
4	2.0	29.0	69.0	-160.710	-48.352	-4.511	-8.773	-280.110	-8.826	-167.823
5	2.0	39.0	59.0	-160.357	-48.100	-4.656	-8.742	-279.731	-8.809	-167.325
6	2.0	49.0	49.0	-159.807	-47.832	-4.898	-8.709	-279.109	-8.794	-166.532
7	2.0	59.0	39.0	-158.484	-47.391	-5.525	-8.674	-277.526	-8.803	-164.583
8	2.0	69.0	29.0	-8.438	-5.797	-88.677	-8.675	-101.203	-48.865	-34.260
9	2.0	79.0	19.0	-13.092	-4.670	-91.499	-9.531	-97.007	-50.139	-36.658
10	2.0	89.0	9.0	-14.260	-4.409	-92.894	-10.220	-94.946	-50.523	-37.306
11	2.0	96.0	2.0	-14.757	-4.304	-94.691	-10.612	-92.269	-50.706	-37.593
12	10.0	2.0	88.0	-159.384	-49.776	-4.401	-8.805	-280.400	-8.816	-168.216
13	10.0	10.0	80.0	-159.186	-48.910	-4.477	-8.782	-280.199	-8.812	-167.942
14	10.0	20.0	70.0	-158.867	-48.469	-4.606	-8.752	-279.862	-8.798	-167.494
15	10.0	30.0	60.0	-158.396	-48.132	-4.809	-8.719	-279.338	-8.782	-166.820
16	10.0	40.0	50.0	-157.477	-47.741	-5.234	-8.685	-278.257	-8.776	-165.475
17	10.0	50.0	40.0	0.474	-8.143	-84.239	-8.646	-107.860	-46.517	-29.564
18	10.0	60.0	30.0	1.006	-7.910	-84.745	-8.606	-107.081	-46.672	-29.952
19	10.0	70.0	20.0	0.730	-7.679	-85.254	-8.562	-106.296	-46.814	-30.327
20	10.0	80.0	10.0	-10.703	-4.809	-91.640	-9.117	-96.739	-49.777	-36.158
21	10.0	88.0	2.0	-12.156	-4.477	-94.045	-9.884	-93.164	-50.231	-36.946
22	20.0	2.0	78.0	-158.096	-49.597	-4.639	-8.745	-279.777	-8.759	-167.384
23	20.0	10.0	70.0	-157.703	-48.681	-4.809	-8.719	-279.338	-8.755	-166.820
24	20.0	20.0	60.0	-156.784	-48.088	-5.234	-8.685	-278.257	-8.749	-165.475
25	20.0	30.0	50.0	1.444	-8.386	-84.343	-8.646	-107.704	-46.275	-29.080
26	20.0	40.0	40.0	2.249	-8.220	-84.818	-8.606	-106.973	-46.360	-29.329
27	20.0	50.0	30.0	2.674	-8.165	-85.130	-8.562	-106.482	-46.330	-29.353
28	20.0	60.0	20.0	3.056	-8.147	-85.477	-8.514	-105.939	-46.253	-29.292
29	20.0	70.0	10.0	3.538	-8.176	-86.011	-8.461	-105.110	-46.119	-29.130
30	22.0	76.0	2.0	15.974	-11.218	-92.827	-9.208	-95.260	-44.566	-24.841
31	18.0	80.0	2.0	-7.206	-5.459	-91.646	-8.516	-96.653	-48.812	-34.548
32	30.0	2.0	68.0	-156.019	-49.146	-5.407	-8.678	-277.822	-8.698	-164.944
33	30.0	10.0	60.0	3.272	-8.842	-85.044	-8.645	-106.653	-45.820	-28.164
34	30.0	20.0	50.0	15.932	-11.641	-91.404	-8.605	-97.094	-42.938	-23.943
35	30.0	30.0	40.0	16.172	-11.589	-91.587	-8.557	-96.794	-42.894	-23.915
36	30.0	40.0	30.0	16.156	-11.493	-91.670	-8.504	-96.644	-42.883	-23.788
37	30.0	50.0	20.0	16.133	-11.406	-91.801	-8.444	-96.417	-42.850	-23.623
38	30.0	60.0	10.0	16.106	-11.323	-92.067	-8.376	-95.984	-42.797	-23.392
39	30.0	68.0	2.0	16.084	-11.257	-92.802	-8.314	-94.850	-42.739	-23.037
40	40.0	10.0	50.0	16.664	-12.354	-91.702	-8.537	-96.612	-42.091	-23.977
41	40.0	20.0	40.0	16.407	-11.859	-91.630	-8.419	-96.693	-42.475	-23.823
42	40.0	30.0	30.0	16.309	-11.656	-91.662	-8.347	-96.613	-42.551	-23.657
43	40.0	40.0	20.0	16.243	-11.511	-91.760	-8.263	-96.430	-42.552	-23.462
44	40.0	50.0	10.0	16.189	-11.389	-91.996	-8.263	-96.034	-42.506	-23.193
45	40.0	58.0	2.0	16.150	-11.296	-92.706	-8.184	-94.930	-42.442	-22.779

TABLE 16b

300°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.8E-02	1.7E-01	2.6E-01	3.3E-01	7.2E-01	7.1E-01	0.
H2	4.2E-04	3.6E-04	4.3E-07	3.3E-01	4.0E-04	7.3E-07	4.0E-39
O2	0.	0.	0.	0.	0.	0.	5.0E-01
WATER	6.9E-01	3.3E-01	4.5E-07	3.3E-01	1.1E-01	4.8E-07	2.5E-01
CO	1.8E-09	6.0E-09	7.7E-06	1.6E-17	6.6E-09	4.5E-06	0.
CO2	2.7E-01	5.0E-01	7.3E-01	1.4E-12	1.7E-01	2.6E-01	2.5E-01
BENZENE	0.	3.2E-35	1.0E-07	0.	9.5E-32	3.4E-07	0.
NAPHTHALENE	0.	0.	4.6E-08	0.	0.	2.0E-07	0.
ASPHALT	0.	0.	4.8E-03	0.	0.	2.8E-02	0.
ACETYLENE	0.	1.2E-38	1.8E-29	0.	1.8E-37	2.7E-29	0.
ETHYLENE	1.2E-22	3.1E-21	5.3E-15	1.5E-26	4.8E-20	1.4E-14	0.
ETHANE	3.7E-12	8.1E-11	1.7E-07	3.5E-13	1.4E-09	7.3E-07	0.
FORMIC ACID	5.9E-16	9.4E-16	1.6E-18	2.4E-24	3.4E-16	1.0E-18	0.
ACETIC ACID	2.4E-15	1.9E-14	4.4E-14	1.1E-25	2.8E-14	4.3E-14	0.
FORMALDEHYDE	2.4E-21	6.9E-21	1.0E-20	1.6E-26	8.3E-21	1.0E-20	0.
ACETALDEHYDE	3.1E-24	4.4E-23	8.9E-20	2.3E-31	2.1E-22	1.4E-19	0.
METHANOL	3.9E-19	9.6E-19	1.7E-21	2.1E-21	1.3E-18	2.9E-21	0.
ETHANOL	2.5E-25	3.0E-24	7.2E-24	1.4E-29	1.6E-23	1.9E-23	0.
N2	1.5E-04	1.7E-04	1.8E-04	6.0E-05	2.2E-04	2.7E-04	1.3E-04
NH3	1.6E-08	1.3E-08	5.5E-13	2.1E-04	1.7E-08	1.5E-12	0.
HCN	5.1E-25	2.9E-24	1.2E-19	1.2E-28	1.3E-23	1.7E-19	0.
NO	0.	0.	0.	0.	0.	0.	6.6E-18
NO2	0.	0.	0.	0.	0.	0.	7.5E-14
N2O	0.	0.	0.	0.	0.	0.	8.5E-25
NITROUS ACID	0.	0.	0.	0.	0.	0.	3.0E-18
NITRIC ACID	0.	0.	0.	0.	0.	0.	4.7E-15
C2N2	0.	0.	0.	0.	0.	0.	0.
HNCO	4.8E-34	1.5E-33	7.1E-32	0.	2.0E-33	6.4E-32	0.
P2	0.	0.	0.	0.	0.	0.	0.
P4O6	7.8E-05	8.4E-05	9.3E-05	8.4E-05	1.1E-04	1.3E-04	0.
P4O10	0.	0.	0.	0.	0.	0.	6.3E-05
PO	0.	0.	0.	0.	0.	0.	0.
PO2	0.	0.	0.	0.	0.	0.	0.
PH2	0.	0.	0.	0.	0.	0.	0.
PH3	0.	0.	0.	1.2E-38	0.	0.	0.
PCl3	0.	0.	0.	0.	0.	0.	0.
POCl3	0.	0.	3.6E-36	0.	0.	6.7E-36	1.8E-33
PSl3	1.2E-38	5.8E-38	1.1E-26	0.	9.3E-37	5.7E-26	0.
Cl2	2.0E-37	2.7E-37	2.8E-34	0.	4.4E-37	3.4E-34	1.1E-04
HCl	3.1E-04	3.4E-04	3.7E-04	3.4E-04	4.5E-04	5.4E-04	2.3E-05
HOCl	0.	0.	0.	0.	0.	0.	4.3E-10
Cl2O	0.	0.	0.	0.	0.	0.	6.0E-23
CH3Cl	9.4E-17	5.2E-16	7.5E-13	1.1E-18	2.7E-15	1.7E-12	0.
CH2Cl2	1.3E-32	8.8E-32	1.2E-25	2.1E-37	5.6E-31	2.3E-25	0.
CHCl3	0.	0.	1.9E-38	0.	0.	3.2E-38	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
COCl2	5.9E-38	2.7E-37	3.5E-31	0.	4.8E-37	2.5E-31	0.
S2	1.0E-22	1.7E-22	8.4E-18	2.0E-28	2.5E-22	2.4E-17	0.
S8	0.	0.	1.2E-32	0.	0.	7.7E-31	0.
H2S	3.1E-04	3.4E-04	9.1E-05	3.4E-04	4.5E-04	2.6E-04	0.
S02	8.4E-24	3.3E-24	9.9E-28	4.3E-33	3.8E-25	6.4E-28	1.6E-14
S03	0.	0.	0.	0.	0.	0.	2.5E-04
COS	2.4E-10	9.9E-10	2.8E-04	2.8E-21	1.3E-09	2.8E-04	0.
CS2	4.4E-20	4.2E-19	2.3E-08	1.2E-30	2.3E-18	6.2E-08	0.
S	0.	0.	0.	0.	0.	0.	0.
SULFURIC ACID	0.	0.	0.	0.	0.	0.	0.
SULFURIC ACID	0.	0.	0.	0.	0.	0.	0.
CYANOGENSULFIDE	0.	0.	0.	0.	0.	0.	6.6E-17
METHANETHIOL	3.6E-15	2.0E-14	7.0E-12	4.3E-17	1.1E-13	3.2E-11	0.
DIMETHYLSULFIDE	5.2E-25	1.4E-23	6.7E-18	6.8E-29	3.0E-22	4.9E-17	0.
DIMET. DISULFIDE	2.9E-32	1.0E-30	1.0E-22	5.1E-39	2.6E-29	1.3E-21	0.
ETHANETHIOL	5.6E-23	1.6E-21	7.2E-16	7.3E-27	3.3E-20	5.3E-15	0.
DIETHYLSULFIDE	0.	7.7E-38	6.2E-26	0.	2.5E-35	1.2E-24	0.
DIETH. DISULFIDE	0.	0.	3.6E-30	0.	0.	1.1E-28	0.
ETHANEDIITHIOL	1.1E-35	3.9E-34	4.1E-26	0.	1.0E-32	5.0E-25	0.
OCTANETHIOL	0.	0.	0.	0.	0.	0.	0.
THIOFORMIC ACID	0.	0.	1.2E-36	0.	0.	2.0E-36	0.
THIOACETIC ACID	0.	0.	9.8E-38	0.	0.	2.6E-37	0.
CYCLOPROP.THIOL	0.	5.3E-38	2.8E-26	0.	4.1E-36	1.9E-25	0.
CYCLOBUTA.THIOL	0.	0.	1.5E-31	0.	0.	1.6E-30	0.
CYCLOCOPENT.THIOL	0.	0.	9.6E-26	0.	0.	1.7E-24	0.
CYCLOHEXA.THIOL	0.	0.	3.4E-28	0.	0.	9.4E-27	0.
M.SULFONIC ACID	0.	0.	0.	0.	0.	0.	0.
E.SULFINIC ACID	5.2E-13	8.1E-12	4.3E-09	4.2E-20	5.2E-11	2.0E-08	0.
THIOPHENENE	3.2E-38	3.6E-35	1.8E-14	0.	9.2E-33	6.6E-14	0.
BENZENETHIOL	0.	0.	2.8E-14	0.	0.	1.6E-13	0.
THIOCYANIC ACID	2.4E-32	1.7E-31	1.6E-24	8.1E-39	9.3E-31	3.9E-24	0.
THIOLGLYCOL	0.	0.	0.	0.	0.	0.	0.
CYSTEINE	0.	0.	0.	0.	0.	0.	0.
METHIONINE	0.	0.	0.	0.	0.	0.	0.

TABLE 17a

300°K AND 0.2 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 25 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS. SYSTEMS CONTAINING LIQUID WATER HAVE BEEN OMITTED.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-161.299	-48.147	-0.837	-5.394	-287.605	-5.393	-172.086
2	2.0	9.0	89.0	-161.177	-47.355	-0.880	-5.376	-287.488	-5.377	-171.921
3	2.0	96.0	2.0	-21.665	-0.850	-94.691	-14.066	-90.542	-47.256	-37.594
4	10.0	2.0	88.0	-159.384	-48.049	-0.947	-5.351	-287.308	-5.350	-171.670
5	10.0	10.0	80.0	-159.186	-47.183	-1.023	-5.328	-287.107	-5.330	-171.397
6	10.0	88.0	2.0	-19.064	-1.023	-94.044	-13.247	-91.437	-46.779	-36.947
7	20.0	2.0	78.0	-158.096	-47.870	-1.185	-5.291	-286.684	-5.291	-170.838
8	20.0	10.0	70.0	-157.703	-46.954	-1.355	-5.265	-286.245	-5.269	-170.275
9	20.0	70.0	10.0	3.536	-6.448	-82.557	-5.007	-108.565	-40.938	-25.679
10	22.0	76.0	2.0	15.247	-9.309	-89.009	-5.754	-99.260	-39.568	-22.178
11	18.0	80.0	2.0	-14.101	-2.008	-91.639	-9.856	-94.936	-45.357	-34.541
12	30.0	2.0	68.0	-156.019	-47.418	-1.953	-5.224	-284.730	-5.224	-168.398
13	30.0	10.0	60.0	3.272	-7.115	-81.590	-5.191	-110.107	-40.638	-24.713
14	30.0	20.0	50.0	15.217	-9.735	-87.592	-5.152	-101.084	-37.937	-20.568
15	30.0	30.0	40.0	15.445	-9.680	-87.770	-5.103	-100.793	-37.895	-20.676
16	30.0	40.0	30.0	15.429	-9.585	-87.852	-5.050	-100.643	-37.885	-20.744
17	30.0	50.0	20.0	15.405	-9.497	-87.984	-4.990	-100.416	-37.852	-20.781
18	30.0	60.0	10.0	15.379	-9.414	-88.249	-4.922	-99.983	-37.800	-20.729
19	30.0	68.0	2.0	15.357	-9.348	-88.985	-4.860	-98.849	-37.742	-20.372
20	40.0	10.0	50.0	15.937	-10.446	-87.885	-5.084	-100.611	-37.092	-20.252
21	40.0	20.0	40.0	15.680	-9.950	-87.812	-5.028	-100.692	-37.476	-20.262
22	40.0	30.0	30.0	15.582	-9.747	-87.844	-4.965	-100.613	-37.554	-20.337
23	40.0	40.0	20.0	15.516	-9.603	-87.942	-4.893	-100.430	-37.554	-20.411
24	40.0	50.0	10.0	15.462	-9.480	-88.179	-4.809	-100.033	-37.509	-20.411
25	40.0	58.0	2.0	15.423	-9.388	-88.889	-4.730	-98.929	-37.443	-20.090

TABLE 17b

300°K AND 0.2 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH THREE SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS. SYSTEMS CONTAINING LIQUID WATER HAVE BEEN OMITTED.

COMPOUND	C	E	F
METHANE	7.2E-01	2.6E-01	7.1E-01
H2	1.3E-05	2.0E-08	3.3E-08
O2	0.	0.	0.
WATER	1.1E-01	9.4E-07	9.9E-07
CO	2.1E-10	1.7E-07	9.8E-08
CO2	1.7E-01	7.3E-01	2.6E-01
BENZENE	3.0E-30	1.2E-07	4.0E-07
NAPHTHALENE	0.	1.4E-07	5.9E-07
ASPHALT	0.	4.8E-03	2.8E-02
ACETYLENE	0.	1.9E-31	2.9E-31
ETHYLENE	4.8E-20	2.6E-15	6.6E-15
ETHANE	4.4E-08	3.7E-06	1.6E-05
FORMIC ACID	1.1E-14	7.4E-17	4.5E-17
ACETIC ACID	2.8E-11	4.4E-11	4.3E-11
FORMALDEHYDE	8.3E-21	1.0E-20	1.0E-20
ACETALDEHYDE	6.7E-21	1.9E-18	3.1E-18
METHANOL	4.0E-17	7.0E-20	1.3E-19
ETHANOL	1.6E-20	7.2E-21	1.9E-20
N2	2.2E-04	1.8E-04	2.7E-04
NH3	9.5E-08	5.3E-12	1.4E-11
HCN	2.2E-24	1.2E-20	1.8E-20
NO	0.	0.	0.
NO2	0.	0.	0.
N2O	0.	0.	0.
NITROUS ACID	0.	0.	0.
NITRIC ACID	0.	0.	0.
C2N2	0.	0.	0.
HNC	1.1E-32	3.3E-31	3.0E-31
P2	0.	0.	0.
P4O6	1.1E-04	9.3E-05	1.3E-04
P4O10	0.	0.	0.
PO	0.	0.	0.
PO2	0.	0.	0.
PH2	0.	0.	0.
PH3	0.	0.	0.
PCL3	0.	6.9E-39	2.1E-38
POCL3	8.1E-38	9.7E-33	1.8E-32
PSCL3	5.2E-33	1.7E-23	4.8E-23
CL2	1.4E-35	6.1E-33	7.3E-33
HCL	4.5E-04	3.7E-04	5.4E-04
HOCL	0.	0.	0.
CL2O	0.	0.	0.
CH3CL	8.6E-14	1.6E-11	3.8E-11
CH2CL2	5.6E-28	5.7E-23	1.1E-22
CHCL3	0.	2.1E-34	3.3E-34
CCL4	0.	0.	0.
COCL2	4.8E-34	1.7E-28	1.2E-28
S2	2.5E-22	5.5E-18	4.9E-18
S8	0.	2.1E-24	1.4E-24
H2S	4.5E-04	1.0E-04	1.7E-04
S02	1.2E-23	5.2E-26	1.9E-26
SO3	0.	0.	0.
COS	1.3E-09	1.6E-04	8.7E-05
CS2	2.2E-18	7.4E-09	6.2E-09
S	0.	0.	0.
SULFUROUS ACID	0.	0.	0.
SULFURIC ACID	0.	0.	0.
CYANOGENSULFIDE	0.	0.	0.
METHANETHIOL	3.3E-12	1.8E-10	4.6E-10
DIMETHYLSULFIDE	3.0E-19	3.7E-15	1.5E-14
DIMET.DISULFIDE	8.1E-25	1.5E-18	5.8E-18
ETHANETHIOL	3.2E-17	4.0E-13	1.7E-12
DIETHYLSULFIDE	2.5E-29	1.7E-20	1.8E-19
DIETH.DISULFIDE	2.5E-34	2.5E-23	2.5E-22
ETHANEODITHIOL	3.1E-28	5.0E-22	2.3E-21
OCTANETHIOL	0.	3.9E-33	2.6E-31
THIOFORMIC ACID	1.6E-37	3.1E-35	2.9E-35
THIODACETIC ACID	0.	5.5E-35	8.2E-35
CYCLOPROP.THIOL	4.1E-33	7.5E-24	2.9E-23
CYCLOBUTA.THIOL	0.	8.8E-28	5.4E-27
CYCLOPENT.THIOL	1.3E-34	1.3E-20	1.2E-19
CYCLOHEXA.THIOL	4.2E-38	9.7E-22	1.5E-20
M-SULFONIC ACID	0.	0.	0.
E-SULFINIC ACID	1.6E-06	1.1E-04	2.6E-04
THIOPHENE	2.9E-31	5.1E-14	1.1E-13
BENZENETHIOL	1.4E-37	8.7E-13	2.7E-12
THIOCYANIC ACID	5.2E-30	4.1E-24	5.7E-24
THIOLYGLYCOL	0.	4.4E-38	1.1E-37
CYSTEINE	0.	0.	0.
METHIONINE	0.	0.	0.

TABLE 18a

300°K AND 20 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 13 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS. SYSTEMS CONTAINING LIQUID WATER HAVE BEEN OMITTED.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	D	C	H	O	N	P	Cl	S
1	22.0	76.0	2.0	14.762	-8.036	-86.465	-3.451	-101.925	-36.232	-25.952
2	30.0	20.0	50.0	14.736	-8.464	-85.049	-2.849	-103.747	-34.599	-23.543
3	30.0	30.0	40.0	14.961	-8.408	-85.225	-2.800	-103.459	-34.560	-24.058
4	30.0	40.0	30.0	14.945	-8.312	-85.307	-2.747	-103.309	-34.547	-24.412
5	30.0	50.0	20.0	14.921	-8.225	-85.438	-2.687	-103.082	-34.515	-24.637
6	30.0	60.0	10.0	14.895	-8.142	-85.704	-2.619	-102.649	-34.465	-24.681
7	30.0	68.0	2.0	14.872	-8.076	-86.461	-2.557	-101.514	-34.407	-24.175
8	40.0	10.0	50.0	15.457	-9.181	-85.342	-2.781	-103.274	-33.747	-20.327
9	40.0	20.0	40.0	15.196	-8.679	-85.267	-2.725	-103.358	-34.143	-22.717
10	40.0	30.0	30.0	15.098	-8.475	-85.299	-2.662	-103.279	-34.216	-23.582
11	40.0	40.0	20.0	15.032	-8.330	-85.397	-2.590	-103.096	-34.216	-24.075
12	40.0	50.0	10.0	14.978	-8.208	-85.634	-2.506	-102.700	-34.173	-24.299
13	40.0	58.0	2.0	14.938	-8.115	-86.345	-2.427	-101.594	-34.110	-23.904

TABLE 18b  
 300°K AND 20 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS  
 IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H,  
 O, N, P, S, AND CI WITH TWO SELECTED RELATIVE ABUNDANCE  
 RATIOS OF C, H, AND O. N, P, S, AND CI CONSTITUTE 0.01%  
 OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS. SYSTEMS  
 CONTAINING LIQUID WATER HAVE BEEN OMITTED.

COMPOUND	C	F
METHANE	2.6E-01	7.1E-01
H2	2.5E-09	4.2E-09
O2	0.	0.
WATER	1.5E-06	1.6E-06
CO	1.3E-08	7.7E-09
CO2	7.3E-01	2.6E-01
BENZENE	1.4E-07	4.6E-07
NAPHTHALENE	2.8E-07	1.2E-06
ASPHALT	4.9E-03	2.8E-02
ACETYLENE	9.2E-33	1.4E-32
ETHYLENE	1.6E-15	4.0E-15
ETHANE	2.9E-05	1.3E-04
FORMIC ACID	9.5E-16	5.8E-16
ACETIC ACID	4.4E-09	4.3E-09
FORMALDEHYDE	1.0E-20	1.0E-20
ACETALDEHYDE	1.5E-17	2.4E-17
METHANOL	1.0E-18	1.7E-18
ETHANOL	7.2E-19	1.9E-18
N2	1.8E-04	2.7E-04
NH3	2.4E-11	6.5E-11
HCN	2.6E-21	3.9E-21
NO	0.	0.
NO2	0.	0.
N2O	0.	0.
NITROUS ACID	0.	0.
NITRIC ACID	0.	0.
C2N2	0.	0.
HNCO	9.3E-31	8.5E-31
P2	0.	0.
P4O6	9.3E-05	1.3E-04
P4O10	0.	0.
PO	0.	0.
PO2	0.	0.
PH2	0.	0.
PH3	0.	0.
PCl3	1.1E-37	3.2E-37
POCl3	1.9E-30	3.5E-30
PSlCl3	8.9E-24	1.4E-23
Cl2	4.8E-32	5.8E-32
HCl	3.8E-04	5.4E-04
HOCl	0.	0.
Cl2O	0.	0.
CH3Cl	1.3E-10	3.0E-10
CH2Cl2	3.5E-21	6.8E-21
CHCl3	1.0E-31	1.6E-31
CCL4	0.	0.
COCl2	1.1E-26	7.4E-27
S2	6.3E-23	1.8E-23
S8	3.7E-38	0.
H2S	4.5E-07	4.2E-07
SO2	2.9E-27	5.9E-28
SO3	0.	0.
COS	4.2E-07	1.3E-07
CS2	5.2E-14	1.4E-14
S	0.	0.
SULFUROUS ACID	0.	0.
SULFURIC ACID	0.	0.
CYANOGENSULFIDE	0.	0.
METHANETHIOL	6.1E-12	8.9E-12
DIMETHYLSULFIDE	1.0E-15	2.3E-15
DIMETH.SULFIDE	1.4E-20	1.7E-20
ETHANETHIOL	1.1E-13	2.5E-13
DIETHYLSULFIDE	2.8E-19	1.6E-18
DIETH.SULFIDE	1.4E-23	4.4E-23
ETHANEDITHIOL	5.3E-24	6.6E-24
OCTANETHIOL	2.4E-28	9.2E-27
THIOFORMIC ACID	1.0E-36	5.5E-37
THIOACETIC ACID	1.5E-35	1.2E-35
CYCLOPROP.THIOL	1.2E-24	2.7E-24
CYCLOBUTA.THIOL	1.1E-27	3.9E-27
CYCLOPENT.THIOL	1.3E-19	7.0E-19
CYCLOHEXA.THIOL	7.7E-20	6.8E-19
M.SULFONIC ACID	0.	0.
E.SULFINIC ACID	3.7E-04	5.4E-04
THIOPHENE	4.0E-16	4.8E-16
BENZENETHIOL	3.3E-14	5.9E-14
THIOCYANIC ACID	3.1E-26	2.4E-26
THIOLYCOL	1.5E-37	2.1E-37
CYSTEINE	3.0E-38	3.9E-38
METHIONINE	0.	0.

TABLE 19a

500°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-98.160	-30.415	-4.291	-8.848	-152.924	-9.977	-94.810
2	2.0	9.0	89.0	-98.037	-29.622	-4.334	-8.830	-152.808	-10.625	-94.644
3	2.0	19.0	79.0	-97.831	-29.183	-4.409	-8.802	-152.605	-11.010	-94.362
4	2.0	29.0	69.0	-97.571	-28.891	-4.511	-8.773	-152.338	-11.243	-94.001
5	2.0	39.0	59.0	-97.218	-28.640	-4.656	-8.742	-151.958	-11.434	-93.503
6	2.0	49.0	49.0	-96.668	-28.372	-4.898	-8.709	-151.336	-11.633	-92.710
7	2.0	59.0	39.0	-95.345	-27.930	-5.524	-8.674	-149.753	-12.004	-90.762
8	2.0	69.0	29.0	-3.047	-4.943	-51.721	-8.701	-56.239	-35.044	-22.344
9	2.0	79.0	19.0	-1.602	-4.595	-52.872	-8.741	-54.530	-35.471	-23.120
10	2.0	89.0	9.0	-1.889	-4.405	-54.000	-8.783	-52.860	-35.744	-23.581
11	2.0	96.0	2.0	-2.331	-4.304	-55.772	-8.821	-50.220	-35.922	-23.859
12	10.0	2.0	88.0	-96.244	-30.317	-4.401	-8.805	-152.627	-9.980	-94.393
13	10.0	10.0	80.0	-96.047	-29.450	-4.477	-8.782	-152.427	-10.702	-94.120
14	10.0	20.0	70.0	-95.728	-29.008	-4.606	-8.752	-152.089	-11.084	-93.672
15	10.0	30.0	60.0	-95.257	-28.672	-4.809	-8.719	-151.565	-11.353	-92.998
16	10.0	40.0	50.0	-94.338	-28.281	-5.234	-8.685	-150.484	-11.675	-91.654
17	10.0	50.0	40.0	-2.224	-5.248	-51.293	-8.682	-56.869	-34.700	-21.696
18	10.0	60.0	30.0	-0.003	-4.818	-52.533	-8.695	-55.017	-35.159	-22.584
19	10.0	70.0	20.0	0.513	-4.705	-53.026	-8.677	-54.268	-35.234	-22.772
20	10.0	80.0	10.0	0.644	-4.609	-53.614	-8.657	-53.376	-35.292	-22.924
21	10.0	88.0	2.0	0.250	-4.473	-55.185	-8.670	-51.026	-35.451	-23.220
22	20.0	2.0	78.0	-94.957	-30.139	-4.639	-8.745	-152.004	-10.021	-93.561
23	20.0	10.0	70.0	-94.564	-29.221	-4.809	-8.719	-151.565	-10.803	-92.998
24	20.0	20.0	60.0	-93.645	-28.627	-5.234	-8.685	-150.484	-11.328	-91.654
25	20.0	30.0	50.0	-0.470	-5.309	-51.823	-8.678	-56.073	-34.631	-21.566
26	20.0	40.0	40.0	1.369	-5.035	-52.812	-8.663	-54.582	-34.877	-22.092
27	20.0	50.0	30.0	2.101	-5.003	-53.268	-8.623	-53.878	-34.830	-22.069
28	20.0	60.0	20.0	2.793	-5.036	-53.751	-8.572	-53.129	-34.695	-21.900
29	20.0	70.0	10.0	3.824	-5.178	-54.530	-8.505	-51.927	-34.419	-21.481
30	22.0	76.0	2.0	10.376	-6.721	-59.048	-9.228	-45.511	-34.315	-20.222
31	18.0	80.0	2.0	3.349	-5.019	-55.183	-8.486	-50.937	-34.533	-21.760
32	30.0	2.0	68.0	-92.880	-29.687	-5.406	-8.678	-150.050	-10.254	-91.123
33	30.0	10.0	60.0	2.266	-5.652	-52.984	-8.663	-54.325	-34.260	-20.849
34	30.0	20.0	50.0	5.557	-5.980	-54.680	-8.624	-51.760	-33.849	-20.116
35	30.0	30.0	40.0	8.719	-6.636	-56.415	-8.610	-49.151	-33.164	-19.475
36	30.0	40.0	30.0	10.436	-6.988	-57.529	-8.602	-47.476	-32.796	-19.611
37	30.0	50.0	20.0	10.527	-6.930	-57.742	-8.530	-47.121	-32.710	-19.400
38	30.0	60.0	10.0	10.521	-6.845	-58.057	-8.437	-46.602	-32.610	-19.043
39	30.0	68.0	2.0	10.503	-6.765	-59.028	-8.337	-45.095	-32.490	-18.425
40	40.0	10.0	50.0	10.863	-7.564	-57.580	-8.686	-47.443	-32.390	-19.918
41	40.0	20.0	40.0	10.772	-7.330	-57.576	-8.617	-47.413	-32.484	-19.693
42	40.0	30.0	30.0	10.711	-7.172	-57.619	-8.539	-47.310	-32.486	-19.576
43	40.0	40.0	20.0	10.660	-7.041	-57.724	-8.449	-47.107	-32.437	-19.311
44	40.0	50.0	10.0	10.612	-6.916	-57.986	-8.336	-46.658	-32.337	-18.907
45	40.0	58.0	2.0	10.571	-6.807	-58.893	-8.213	-45.235	-32.199	-18.208

TABLE 19b

500°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	1.1E-03	9.5E-02	2.4E-01	2.5E-01	6.2E-01	6.4E-01	0.
H2	1.4E-01	2.1E-01	8.6E-03	5.0E-01	1.6E-01	5.7E-03	3.2E-22
O2	0.	0.	0.	0.	0.	0.	5.0E-01
WATER	5.7E-01	1.9E-01	2.1E-04	2.0E-01	2.6E-02	2.7E-05	2.5E-01
CO	5.2E-04	4.1E-03	1.7E-01	9.0E-04	8.6E-03	2.1E-01	2.4E-24
CO2	2.8E-01	5.0E-01	5.7E-01	4.8E-02	1.9E-01	1.3E-01	2.5E-01
BENZENE	1.2E-33	9.8E-24	9.3E-09	1.6E-24	1.0E-17	1.3E-04	0.
NAPHTHALENE	0.	1.3E-38	2.9E-12	0.	1.8E-28	3.6E-05	0.
ASPHALT	0.	0.	1.5E-18	0.	0.	1.9E-02	0.
ACETYLENE	3.7E-24	7.5E-21	7.4E-16	4.1E-21	7.6E-19	1.8E-14	0.
ETHYLENE	1.7E-16	5.3E-13	2.1E-09	6.8E-13	4.0E-11	3.4E-08	0.
ETHANE	3.8E-13	1.8E-09	2.9E-07	5.5E-09	1.0E-07	3.1E-06	0.
FORMIC ACID	1.7E-12	4.6E-12	2.2E-13	1.0E-12	1.3E-12	3.2E-14	3.5E-33
ACETIC ACID	5.5E-16	8.2E-14	2.4E-13	2.1E-14	2.0E-13	1.5E-13	0.
FORMALDEHYDE	7.3E-14	8.9E-13	1.5E-12	4.5E-13	1.4E-12	1.2E-12	0.
ACETALDEHYDE	5.4E-19	3.6E-16	4.0E-14	2.1E-16	5.0E-15	1.2E-13	0.
METHANOL	2.3E-15	4.2E-14	3.0E-15	5.0E-14	5.0E-14	1.5E-15	0.
ETHANOL	1.8E-22	1.9E-19	8.5E-19	2.6E-19	2.0E-18	1.7E-18	0.
N2	1.4E-04	1.5E-04	1.7E-04	1.5E-04	2.0E-04	2.3E-04	1.3E-04
NH3	4.0E-08	7.8E-08	6.7E-10	2.8E-07	5.9E-08	4.3E-10	4.2E-39
HCN	7.2E-16	3.3E-14	1.1E-11	2.5E-14	3.9E-13	6.4E-11	0.
NO	7.3E-32	1.6E-32	4.7E-34	7.3E-33	3.4E-33	1.1E-34	1.3E-11
NO2	0.	0.	0.	0.	0.	0.	1.5E-11
N2O	0.	0.	0.	0.	0.	0.	4.3E-19
NITROUS ACID	0.	0.	0.	0.	0.	0.	2.4E-15
NITRIC ACID	0.	0.	0.	0.	0.	0.	4.8E-16
C2N2	1.0E-36	1.4E-33	3.7E-27	3.2E-34	2.5E-31	1.9E-25	0.
HNCO	8.7E-16	8.0E-15	7.9E-14	2.9E-15	1.9E-14	8.9E-14	0.
P2	0.	0.	0.	0.	0.	1.7E-37	0.
P4O6	7.2E-05	7.5E-05	8.3E-05	7.6E-05	1.0E-04	1.2E-04	0.
P4O10	0.	0.	0.	0.	0.	0.	6.3E-05
PO	1.9E-33	4.1E-33	2.6E-32	6.2E-33	1.0E-32	6.3E-32	0.
PO2	4.5E-29	2.1E-29	3.6E-30	1.4E-29	9.7E-30	1.7E-30	7.1E-30
PH2	4.3E-28	6.5E-27	6.1E-26	5.1E-26	7.0E-26	5.1E-25	0.
PH3	1.1E-26	2.0E-25	3.8E-25	2.4E-24	1.9E-24	2.6E-24	0.
PCL3	4.1E-37	2.4E-36	9.3E-36	2.3E-36	1.3E-34	6.3E-30	0.
POCL3	1.1E-34	1.4E-34	1.5E-31	6.0E-35	1.4E-33	1.9E-30	5.4E-25
PSCL3	8.7E-34	3.4E-33	1.8E-27	1.4E-33	3.5E-31	1.9E-25	0.
CL2	3.6E-27	2.5E-27	7.8E-26	1.1E-27	6.4E-27	2.4E-25	1.2E-06
HCl	2.9E-04	3.0E-04	3.4E-04	3.0E-04	4.1E-04	4.8E-04	2.5E-04
HOCl	2.6E-29	5.9E-30	1.8E-31	2.7E-30	1.5E-30	4.9E-32	4.3E-09
Cl2O	0.	0.	0.	0.	0.	0.	1.1E-19
CH3Cl	3.4E-15	2.0E-13	1.4E-11	2.3E-13	2.4E-12	7.9E-11	0.
CH2Cl2	1.2E-27	4.6E-26	9.0E-23	2.3E-26	1.0E-24	1.1E-21	0.
CHCl3	0.	6.7E-39	3.6E-34	0.	2.7E-37	9.3E-33	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
COCl2	7.0E-30	3.9E-29	5.1E-26	3.7E-30	2.0E-28	1.8E-25	1.1E-29
S2	7.2E-16	3.2E-16	6.1E-14	6.1E-17	1.1E-15	1.4E-13	0.
S8	0.	0.	0.	0.	0.	0.	0.
SO2	5.7E-17	1.8E-18	1.9E-20	1.6E-19	1.1E-19	1.1E-21	1.1E-07
SO3	6.9E-34	4.8E-36	0.	1.9E-37	5.2E-38	0.	2.5E-04
COS	5.4E-08	2.9E-07	1.7E-04	2.8E-08	1.1E-06	3.1E-04	0.
CS2	2.4E-15	3.9E-14	1.1E-08	3.5E-15	1.5E-12	1.6E-07	0.
SO	6.1E-22	9.0E-23	3.4E-23	1.8E-23	3.0E-23	1.0E-23	6.4E-33
SULFUROUS ACID	0.	0.	0.	0.	0.	0.	2.3E-32
SULFURIC ACID	0.	0.	0.	0.	0.	0.	3.4E-16
CYANOGENSULFIDE	0.	1.1E-38	4.1E-31	0.	3.8E-36	3.3E-29	0.
METHANETHIOL	3.7E-14	2.1E-12	7.5E-11	2.5E-12	2.6E-11	3.0E-10	0.
DIMETHYLSULFIDE	9.6E-24	3.1E-20	6.8E-17	4.0E-20	3.2E-18	1.1E-15	0.
DIMET.DISULFICE	4.1E-31	8.9E-28	2.7E-23	5.1E-28	1.7E-25	6.7E-22	0.
ETHANETHIOL	2.6E-22	8.3E-19	1.8E-15	1.1E-18	8.7E-17	3.0E-14	0.
DIETHYLSULFIDE	0.	4.1E-33	3.7E-26	7.0E-33	3.3E-29	9.5E-24	0.
DIETH.DISULFIDE	0.	0.	2.7E-32	0.	3.3E-36	1.1E-29	0.
ETHANEDIITHIOL	5.5E-33	1.2E-29	3.6E-25	6.7E-30	2.3E-27	8.9E-24	0.
OCTANEDIITHIOL	0.	0.	0.	0.	0.	0.	0.
THIOCROMIC ACID	1.0E-27	8.5E-27	2.0E-25	1.9E-27	2.5E-26	2.4E-25	0.
THIOACETIC ACID	8.9E-34	4.1E-31	6.1E-28	1.0E-31	1.0E-29	2.9E-27	0.
CYCLOPROP.THICL	8.3E-32	9.7E-27	3.3E-20	6.1E-27	1.2E-23	3.3E-18	0.
CYCLOBUTA.THICL	0.	3.3E-34	7.3E-26	2.4E-34	3.6E-30	2.9E-23	0.
CYCLOPENT.THICL	0.	5.8E-37	8.1E-27	4.8E-37	5.4E-32	1.3E-23	0.
CYCLOHEXA.THICL	0.	0.	3.2E-29	0.	3.0E-35	2.0E-25	0.
M.SULFONIC ACID	0.	0.	0.	0.	0.	0.	0.
E-SULFINIC ACID	1.5E-20	1.1E-17	6.4E-16	6.2E-18	2.0E-16	2.0E-15	0.
THIOPHENE	4.1E-31	1.1E-24	1.5E-13	1.5E-25	2.2E-20	1.3E-10	0.
BENZENETHIOL	0.	5.9E-32	7.7E-16	4.3E-33	1.1E-25	1.7E-11	0.
THIOCYANIC ACID	5.2E-23	1.6E-21	7.3E-18	5.3E-22	3.5E-20	6.6E-17	0.
THIOGLYCOL	9.0E-39	6.3E-36	3.8E-34	3.7E-36	1.2E-34	1.2E-33	0.
CYSTEINE	0.	0.	0.	0.	0.	0.	0.
METHICNINE	0.	0.	0.	0.	0.	0.	0.

TABLE 20a

500°K AND 0.2 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

MOLE PERCENTAGE				FREE ENERGIES (F/MOLE)						
NO.	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-98.160	-28.687	-0.837	-5.394	-159.832	-5.637	-98.271
2	2.0	9.0	89.0	-98.037	-27.895	-0.880	-5.376	-159.716	-5.888	-98.105
3	2.0	19.0	79.0	-97.831	-27.456	-0.956	-5.348	-159.513	-6.088	-97.823
4	2.0	29.0	69.0	-97.571	-27.165	-1.057	-5.319	-159.245	-6.237	-97.462
5	2.0	39.0	59.0	-97.218	-26.913	-1.202	-5.288	-158.866	-6.374	-96.963
6	2.0	49.0	49.0	-96.668	-26.645	-1.444	-5.255	-158.244	-6.536	-96.171
7	2.0	59.0	39.0	-95.345	-26.203	-2.070	-5.220	-156.661	-6.825	-94.215
8	2.0	69.0	29.0	-3.220	-2.276	-49.899	-5.210	-57.217	-30.697	-20.665
9	2.0	79.0	19.0	-7.572	-1.216	-52.578	-5.665	-53.234	-31.900	-22.928
10	2.0	89.0	9.0	-8.740	-0.955	-53.972	-6.179	-51.173	-32.285	-23.575
11	2.0	96.0	2.0	-9.237	-0.850	-55.770	-6.483	-48.496	-32.470	-23.863
12	10.0	2.0	88.0	-96.244	-28.589	-0.947	-5.351	-159.535	-5.607	-97.854
13	10.0	10.0	80.0	-96.047	-27.723	-1.023	-5.328	-159.334	-5.902	-97.581
14	10.0	20.0	70.0	-95.728	-27.281	-1.152	-5.298	-158.996	-6.118	-97.133
15	10.0	30.0	60.0	-95.257	-26.945	-1.355	-5.266	-158.473	-6.308	-96.459
16	10.0	40.0	50.0	-94.338	-26.554	-1.780	-5.231	-157.392	-6.568	-95.107
17	10.0	50.0	40.0	-0.689	-3.039	-48.632	-5.196	-59.117	-29.931	-19.140
18	10.0	60.0	30.0	-0.118	-2.804	-49.151	-5.159	-58.321	-30.090	-19.534
19	10.0	70.0	20.0	-0.327	-2.590	-49.639	-5.121	-57.568	-30.224	-19.880
20	10.0	80.0	10.0	-5.184	-1.355	-52.719	-5.393	-52.965	-31.535	-22.425
21	10.0	88.0	2.0	-6.636	-1.023	-55.123	-5.867	-49.391	-31.993	-23.216
22	20.0	2.0	78.0	-94.957	-28.411	-1.185	-5.291	-158.911	-5.579	-97.015
23	20.0	10.0	70.0	-94.564	-27.494	-1.355	-5.265	-158.472	-5.931	-96.460
24	20.0	20.0	60.0	-93.645	-26.900	-1.780	-5.231	-157.392	-6.280	-95.107
25	20.0	30.0	50.0	0.293	-3.277	-48.745	-5.194	-58.948	-29.692	-18.663
26	20.0	40.0	40.0	1.121	-3.109	-49.230	-5.155	-58.200	-29.780	-18.919
27	20.0	50.0	30.0	1.555	-3.055	-49.547	-5.112	-57.704	-29.750	-18.941
28	20.0	60.0	20.0	1.948	-3.039	-49.897	-5.064	-57.154	-29.670	-18.876
29	20.0	70.0	10.0	2.454	-3.073	-50.441	-5.011	-56.313	-29.530	-18.703
30	22.0	16.0	2.0	9.663	-4.806	-54.662	-5.755	-50.353	-29.284	-17.051
31	18.0	80.0	2.0	-1.689	-2.004	-52.727	-5.026	-52.877	-30.574	-20.816
32	30.0	2.0	68.0	-92.880	-27.959	-1.953	-5.224	-156.958	-5.641	-94.576
33	30.0	10.0	60.0	2.142	-3.731	-49.456	-5.192	-57.881	-29.235	-17.751
34	30.0	20.0	50.0	7.244	-4.637	-52.038	-5.153	-53.987	-28.252	-16.158
35	30.0	30.0	40.0	9.859	-5.178	-53.414	-5.106	-51.901	-27.616	-16.176
36	30.0	40.0	30.0	9.845	-5.083	-53.498	-5.053	-51.748	-27.603	-16.043
37	30.0	50.0	20.0	9.822	-4.996	-53.630	-4.992	-51.521	-27.569	-15.871
38	30.0	60.0	10.0	9.796	-4.912	-53.896	-4.924	-51.086	-27.519	-15.627
39	30.0	68.0	2.0	9.774	-4.846	-54.638	-4.861	-49.943	-27.459	-15.249
40	40.0	10.0	50.0	10.345	-5.928	-53.528	-5.088	-51.721	-26.828	-16.257
41	40.0	20.0	40.0	10.097	-5.447	-53.458	-5.032	-51.797	-27.196	-16.096
42	40.0	30.0	30.0	9.999	-5.245	-53.491	-4.968	-51.717	-27.276	-15.923
43	40.0	40.0	20.0	9.934	-5.101	-53.589	-4.896	-51.534	-27.276	-15.718
44	40.0	50.0	10.0	9.880	-4.978	-53.826	-4.812	-51.136	-27.228	-15.435
45	40.0	58.0	2.0	9.840	-4.886	-54.540	-4.732	-50.024	-27.158	-14.997

TABLE 20b

500°K AND 0.2 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.5E-02	1.6E-01	2.6E-01	3.3E-01	7.2E-01	7.0E-01	0.
H2	1.1E-02	1.0E-02	1.6E-04	3.3E-01	1.1E-02	2.7E-04	1.0E-23
O2	0.	0.	0.	0.	0.	0.	5.0E-01
WATER	6.8E-01	3.3E-01	7.9E-05	3.3E-01	1.0E-01	8.3E-05	2.5E-01
CO	3.4E-05	1.2E-04	1.1E-02	6.4E-09	1.3E-04	6.4E-03	7.6E-26
CO2	2.7E-01	5.0E-01	7.2E-01	8.5E-07	1.7E-01	2.6E-01	2.5E-01
BENZENE	6.7E-27	2.3E-22	5.5E-05	3.2E-34	8.4E-19	1.9E-04	0.
NAPHTHALENE	0.	5.2E-36	3.0E-05	0.	4.3E-30	1.3E-04	0.
ASPHALT	0.	0.	4.5E-03	0.	0.	2.7E-02	0.
ACETYLENE	6.6E-24	2.2E-22	1.3E-16	2.4E-26	3.3E-21	2.0E-16	0.
ETHYLENE	2.5E-14	7.1E-13	7.1E-09	2.7E-15	1.2E-11	1.8E-08	0.
ETHANE	4.7E-09	1.1E-07	1.8E-05	1.4E-08	2.0E-06	7.9E-05	0.
FORMIC ACID	1.4E-10	2.2E-10	5.0E-12	1.2E-14	7.9E-11	3.1E-12	1.1E-31
ACETIC ACID	1.7E-11	1.4E-10	3.3E-10	5.0E-16	2.1E-10	3.2E-10	0.
FORMALDEHYDE	4.0E-13	1.2E-12	1.8E-12	2.2E-15	1.4E-12	1.7E-12	0.
ACETALDEHYDE	1.1E-15	1.8E-14	2.7E-12	2.0E-18	8.7E-14	4.2E-12	0.
METHANOL	1.0E-12	2.6E-12	6.4E-14	1.6E-13	3.4E-12	1.1E-13	0.
ETHANOL	3.2E-17	4.4E-16	1.1E-15	1.7E-18	2.3E-15	2.8E-15	0.
N2	1.5E-04	1.7E-04	1.8E-04	1.0E-04	2.2E-04	2.6E-04	1.3E-04
NH3	9.9E-07	8.4E-07	1.8E-09	1.3E-04	1.1E-06	4.7E-09	2.3E-38
HCN	1.0E-15	5.9E-15	4.9E-12	4.9E-17	2.7E-14	7.2E-12	0.
NO	3.4E-32	2.0E-32	3.1E-34	4.7E-34	6.7E-33	2.3E-34	1.3E-11
NO2	0.	0.	0.	0.	0.	0.	4.8E-10
N2O	4.0E-38	2.4E-38	0.	0.	9.4E-39	0.	1.4E-17
NITROUS ACID	0.	0.	0.	0.	0.	0.	4.2E-13
NITRIC ACID	0.	0.	0.	0.	0.	0.	2.7E-12
C2N2	2.3E-35	9.3E-34	4.0E-26	0.	1.8E-32	5.0E-26	0.
HNCO	1.7E-14	5.6E-14	7.1E-13	1.4E-17	7.6E-14	6.4E-13	0.
P2	0.	0.	0.	0.	0.	0.	0.
P4O6	7.7E-05	8.4E-05	9.2E-05	8.4E-05	1.1E-04	1.3E-04	0.
P4O10	1.3E-37	1.3E-38	0.	0.	0.	0.	6.3E-05
PO	2.9E-36	4.0E-36	3.3E-35	2.3E-35	7.8E-36	4.6E-35	0.
PO2	9.7E-31	7.3E-31	9.3E-32	1.3E-31	4.3E-31	8.0E-32	7.1E-33
PH2	3.8E-30	8.2E-30	7.2E-29	5.2E-26	5.9E-29	2.8E-28	0.
PH3	8.6E-28	1.8E-27	1.9E-27	6.4E-23	1.3E-26	9.6E-27	0.
PCL3	7.2E-35	2.8E-34	1.0E-28	2.7E-34	3.9E-33	3.0E-28	0.
POCL3	2.7E-31	5.8E-31	3.2E-27	1.7E-32	2.4E-30	5.9E-27	5.0E-23
PSCL3	1.9E-30	9.5E-30	5.3E-23	2.8E-31	1.7E-28	2.8E-22	0.
CL2	5.0E-26	6.8E-26	5.2E-24	2.0E-27	1.1E-25	6.2E-24	2.4E-05
HCL	3.1E-04	3.4E-04	3.7E-04	3.4E-04	4.5E-04	5.3E-04	2.0E-04
HOCL	4.0E-28	2.4E-28	4.0E-30	7.3E-30	9.4E-29	3.5E-30	1.1E-07
CL2O	0.	0.	0.	0.	0.	0.	7.3E-17
CH3CL	1.4E-12	8.1E-12	8.9E-10	5.0E-13	4.4E-11	2.0E-09	0.
CH2CL2	6.3E-24	4.5E-23	3.4E-19	8.3E-26	3.0E-22	6.6E-19	0.
CHCl3	1.8E-35	1.6E-34	8.2E-29	8.6E-39	1.3E-33	1.3E-28	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
COCL2	6.5E-27	2.9E-26	2.1E-22	4.9E-32	5.5E-26	1.5E-22	6.9E-27
S2	1.2E-16	1.8E-16	4.4E-14	1.7E-19	2.8E-16	1.3E-13	0.
S8	0.	0.	6.1E-38	0.	0.	4.9E-36	0.
H2S	3.1E-04	3.4E-04	8.4E-05	3.4E-04	4.5E-04	2.5E-04	0.
SU2	1.5E-16	5.6E-17	2.0E-19	1.6E-21	6.2E-18	1.3E-19	3.5E-09
SU3	2.6E-32	5.4E-33	3.0E-37	0.	1.8E-34	1.2E-37	2.5E-04
COS	4.7E-08	2.0E-07	2.9E-04	3.3E-13	2.7E-07	2.9E-04	0.
CS2	1.8E-15	1.7E-14	2.6E-08	2.8E-20	1.0E-13	7.3E-08	0.
SO	1.1E-22	7.7E-23	1.8E-23	7.1E-26	2.9E-23	2.0E-23	6.3E-36
SULFURIC ACID	8.4E-38	1.5E-38	0.	0.	0.	0.	7.2E-31
SULFURIC ACID	0.	0.	0.	0.	0.	0.	3.4E-13
CYANOGENSULFIDE	0.	1.8E-37	1.2E-28	0.	4.3E-36	2.6E-28	0.
METHANETHIOL	1.5E-11	8.8E-11	2.2E-09	5.4E-12	4.8E-10	1.0E-08	0.
DIMETHYLSULFIDE	1.5E-18	4.6E-17	1.1E-13	1.7E-19	1.0E-15	8.6E-13	0.
DIMETH.SULSFIDE	8.4E-25	3.2E-23	1.2E-18	3.6E-27	8.8E-22	1.6E-17	0.
ETHANETHIOL	4.1E-17	1.2E-15	3.1E-12	4.7E-18	2.8E-14	2.3E-11	0.
DIETHYLSULFIDE	9.8E-30	8.4E-27	2.1E-19	1.2E-31	3.1E-24	3.9E-18	0.
DIETH.SULSFIDE	1.0E-35	1.1E-32	4.1E-24	0.	5.0E-30	1.4E-22	0.
ETHANEDIETHIOL	1.1E-26	4.3E-25	1.6E-20	4.8E-29	1.2E-23	2.1E-19	0.
OCTANETHIOL	0.	0.	1.2E-32	0.	0.	1.5E-30	0.
THIOFORMIC ACID	7.4E-26	2.7E-25	6.3E-24	1.5E-29	4.1E-25	1.1E-23	0.
THIOACETIC ACID	2.4E-29	4.7E-28	1.1E-24	1.6E-33	2.9E-27	3.0E-24	0.
CYCLOPRCP.THICL	6.1E-26	1.1E-23	1.7E-16	7.8E-29	9.6E-22	1.2E-15	0.
CYCLOBUTA.THICL	1.5E-32	1.4E-29	2.2E-20	6.1E-36	5.0E-27	2.5E-19	0.
CYCLOPENT.THICL	1.8E-34	9.3E-31	1.4E-19	2.4E-38	1.3E-27	2.5E-18	0.
CYCLOHEXA.THICL	7.5E-38	2.1E-33	3.2E-20	0.	1.2E-29	9.2E-19	0.
M.SULFONIC ACID	5.2E-38	5.0E-38	0.	0.	7.2E-39	0.	0.
E.SULFINIC ACID	3.4E-14	5.7E-13	2.1E-11	6.5E-17	3.8E-12	9.9E-11	0.
THIOPHENE	1.7E-26	2.2E-23	1.3E-10	8.3E-33	6.6E-21	5.2E-10	0.
BENZENETHIOL	7.8E-34	3.3E-29	1.2E-10	0.	1.5E-25	7.2E-10	0.
THIOCYANIC ACID	9.3E-22	6.9E-21	8.9E-17	1.7E-24	3.9E-20	2.3E-16	0.
THIOLYCOL	2.0E-32	3.4E-31	1.3E-29	3.9E-35	2.3E-30	6.0E-29	0.
CYSTEINE	0.	2.0E-38	9.3E-36	0.	1.8E-37	3.9E-35	0.
METHICNINE	0.	0.	0.	0.	0.	0.	0.

TABLE 2la

500°K AND 20 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\bar{F}_i/RT$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MCLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-98.160	-27.535	1.466	-3.092	-164.437	-3.167	-100.566
2	2.0	9.0	89.0	-98.037	-26.743	1.423	-3.073	-164.321	-3.240	-100.401
3	2.0	19.0	79.0	-97.831	-26.304	1.347	-3.046	-164.118	-3.298	-100.118
4	2.0	29.0	69.0	-97.571	-26.013	1.246	-3.017	-163.850	-3.343	-99.757
5	2.0	39.0	59.0	-97.218	-25.761	1.100	-2.986	-163.471	-3.389	-99.259
6	2.0	49.0	49.0	-96.668	-25.493	0.858	-2.953	-162.849	-3.456	-98.466
7	2.0	59.0	39.0	-95.345	-25.052	0.232	-2.918	-161.266	-3.540	-96.517
8	2.0	69.0	29.0	-7.507	-0.045	-49.748	-3.960	-56.291	-28.318	-20.522
9	2.0	79.0	19.0	-12.176	1.087	-52.577	-7.373	-52.083	-29.596	-22.929
10	2.0	89.0	9.0	-13.345	1.348	-53.972	-8.281	-50.021	-29.982	-23.576
11	2.0	96.0	2.0	-13.842	1.452	-55.770	-8.673	-47.344	-30.167	-23.864
12	10.0	2.0	88.0	-96.244	-27.437	1.356	-3.048	-164.140	-3.128	-100.150
13	10.0	10.0	80.0	-96.047	-26.571	1.280	-3.025	-163.939	-3.215	-99.876
14	10.0	20.0	70.0	-95.728	-26.130	1.151	-2.995	-163.602	-3.280	-99.428
15	10.0	30.0	60.0	-95.257	-25.793	0.948	-2.963	-163.078	-3.346	-98.754
16	10.0	40.0	50.0	-94.338	-25.402	0.522	-2.928	-161.997	-3.463	-97.410
17	10.0	50.0	40.0	-0.666	-1.875	-46.344	-2.895	-61.398	-26.487	-16.860
18	10.0	60.0	30.0	-0.131	-1.641	-46.850	-2.860	-60.619	-26.641	-17.247
19	10.0	70.0	20.0	-0.402	-1.411	-47.357	-2.826	-59.835	-26.785	-17.622
20	10.0	80.0	10.0	-9.787	0.948	-52.718	-6.732	-51.815	-29.232	-22.427
21	10.0	88.0	2.0	-11.241	1.280	-55.123	-7.854	-48.239	-29.693	-23.217
22	20.0	2.0	78.0	-94.957	-27.259	1.118	-2.989	-163.516	-3.079	-99.317
23	20.0	10.0	70.0	-94.564	-26.343	0.948	-2.963	-163.078	-3.186	-98.754
24	20.0	20.0	60.0	-93.645	-25.749	0.522	-2.928	-161.997	-3.314	-97.410
25	20.0	30.0	50.0	0.305	-2.117	-46.448	-2.892	-61.241	-26.245	-16.376
26	20.0	40.0	40.0	1.112	-1.951	-46.923	-2.853	-60.508	-26.328	-16.625
27	20.0	50.0	30.0	1.537	-1.896	-47.236	-2.810	-60.017	-26.298	-16.650
28	20.0	60.0	20.0	1.921	-1.878	-47.583	-2.762	-59.474	-26.221	-16.590
29	20.0	70.0	10.0	2.404	-1.907	-48.118	-2.709	-58.645	-26.087	-16.426
30	22.0	76.0	2.0	9.178	-3.534	-52.104	-3.451	-53.038	-25.950	-14.878
31	18.0	80.0	2.0	-6.278	0.295	-52.718	-4.463	-51.739	-28.269	-20.809
32	30.0	2.0	68.0	-92.880	-26.807	0.350	-2.921	-161.562	-3.055	-96.878
33	30.0	10.0	60.0	2.135	-2.573	-47.149	-2.889	-60.189	-25.788	-15.459
34	30.0	20.0	50.0	8.993	-3.921	-50.609	-2.849	-54.980	-24.360	-13.762
35	30.0	30.0	40.0	9.377	-3.905	-50.864	-2.801	-54.573	-24.279	-13.764
36	30.0	40.0	30.0	9.362	-3.810	-50.947	-2.747	-54.422	-24.267	-13.658
37	30.0	50.0	20.0	9.338	-3.723	-51.078	-2.688	-54.195	-24.235	-13.522
38	30.0	60.0	10.0	9.312	-3.639	-51.344	-2.619	-53.762	-24.181	-13.333
39	30.0	68.0	2.0	9.290	-3.573	-52.080	-2.557	-52.628	-24.122	-13.056
40	40.0	10.0	50.0	9.870	-4.670	-50.979	-2.781	-54.390	-23.475	-13.784
41	40.0	20.0	40.0	9.613	-4.175	-50.907	-2.726	-54.471	-23.858	-13.623
42	40.0	30.0	30.0	9.515	-3.972	-50.939	-2.663	-54.392	-23.935	-13.491
43	40.0	40.0	20.0	9.449	-3.828	-51.037	-2.591	-54.209	-23.937	-13.329
44	40.0	50.0	10.0	9.395	-3.706	-51.273	-2.507	-53.812	-23.891	-13.107
45	40.0	58.0	2.0	9.356	-3.613	-51.983	-2.428	-52.708	-23.825	-12.781

TABLE 21b

500°K AND 20 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.8E-02	1.7E-01	2.6E-01	3.3E-01	7.2E-01	7.1E-01	0.
H2	1.2E-03	1.0E-03	2.0E-05	3.3E-01	1.1E-03	3.5E-05	1.0E-24
O2	0.	0.	0.	0.	0.	0.	5.0E-01
WATER	6.9E-01	3.3E-01	1.3E-04	3.3E-01	1.1E-01	1.4E-04	2.5E-01
CO	3.5E-06	1.2E-05	8.7E-04	6.5E-13	1.3E-05	5.0E-04	7.6E-27
CO2	2.7E-01	5.0E-01	7.3E-01	8.5E-11	1.7E-01	2.6E-01	2.5E-01
BENZENE	8.3E-26	2.3E-21	6.3E-05	0.	6.8E-18	2.1E-04	0.
NAPHTHALENE	0.	5.0E-34	6.4E-05	0.	2.9E-28	2.8E-04	0.
ASPHALT	0.	0.	4.8E-03	0.	0.	2.8E-02	0.
ACETYLENE	7.1E-25	2.1E-23	6.5E-18	2.4E-30	3.1E-22	9.7E-18	0.
ETHYLENE	2.8E-14	7.2E-13	4.4E-09	2.7E-17	1.1E-11	1.1E-08	0.
ETHANE	5.3E-08	1.2E-06	1.4E-04	1.4E-08	2.0E-05	6.2E-04	0.
FORMIC ACID	1.4E-09	2.2E-09	6.5E-11	1.2E-16	8.1E-10	4.0E-11	1.1E-30
ACETIC ACID	1.8E-09	1.5E-08	3.3E-08	5.0E-18	2.1E-08	3.2E-08	0.
FORMALDEHYDE	4.1E-13	1.2E-12	1.8E-12	2.2E-21	1.4E-12	1.8E-12	0.
ACETALDEHYDE	1.2E-14	1.8E-13	2.1E-11	2.0E-20	8.6E-13	3.3E-11	0.
METHANOL	1.1E-11	2.7E-11	8.2E-13	1.6E-13	3.5E-11	1.4E-12	0.
ETHANOL	3.6E-15	4.5E-14	1.1E-13	1.7E-18	2.3E-13	2.8E-13	0.
N2	1.5E-04	1.7E-04	1.8E-04	7.1E-08	2.2E-04	2.7E-04	1.3E-04
NH3	3.3E-06	2.7E-06	8.1E-09	3.3E-04	3.6E-06	2.2E-08	7.4E-38
HCN	3.3E-16	1.9E-15	1.1E-12	1.3E-20	8.2E-15	1.6E-12	0.
NO	3.4E-32	2.0E-32	4.0E-34	1.2E-36	6.9E-33	3.0E-34	1.3E-11
NO2	0.	0.	0.	0.	0.	0.	4.8E-09
N2O	3.9E-37	2.4E-37	0.	0.	9.6E-38	0.	1.4E-16
NITROUS ACID	0.	0.	0.	0.	0.	0.	1.3E-11
NITRIC ACID	0.	0.	0.	0.	0.	0.	8.6E-10
C2N2	2.4E-35	9.1E-34	1.5E-26	0.	1.6E-32	1.9E-26	0.
HNCO	5.6E-14	1.8E-13	2.0E-12	3.8E-21	2.4E-13	1.8E-12	0.
P2	0.	0.	0.	0.	0.	0.	0.
P4O6	7.8E-05	8.4E-05	9.3E-05	8.4E-05	1.1E-04	1.3E-04	0.
P4O10	1.2E-33	1.3E-34	0.	0.	1.4E-36	0.	6.3E-05
PO	2.9E-38	4.0E-38	2.9E-37	7.2E-37	7.7E-38	4.1E-37	0.
PO2	9.6E-32	7.4E-32	1.0E-32	4.1E-33	4.3E-32	9.0E-33	7.1E-35
PH2	4.0E-32	8.3E-32	6.3E-31	1.6E-25	5.9E-31	2.4E-30	0.
PH3	2.9E-29	5.6E-29	6.0E-29	2.0E-21	4.1E-28	3.0E-28	0.
PCl3	2.2E-33	8.8E-33	1.6E-27	8.6E-33	1.2E-31	4.7E-27	0.
POCl3	8.3E-29	1.8E-28	6.3E-25	5.5E-31	7.4E-28	1.2E-24	2.5E-22
PSCl3	6.0E-28	3.0E-27	9.1E-21	8.8E-30	4.8E-26	4.2E-20	0.
Cl2	4.9E-25	6.8E-25	4.1E-23	2.0E-27	1.1E-24	5.0E-23	7.1E-05
HCl	3.1E-04	3.4E-04	3.7E-04	3.4E-04	4.5E-04	5.4E-04	1.1E-04
HOCl	4.0E-27	2.4E-27	5.1E-29	7.3E-30	9.7E-28	4.6E-29	5.9E-07
Cl2O	0.	0.	0.	0.	0.	0.	2.1E-15
CH3Cl	1.5E-11	8.2E-11	7.1E-09	5.0E-13	4.3E-10	1.6E-08	0.
CH2Cl2	6.5E-22	4.5E-21	2.1E-17	8.3E-26	2.9E-20	4.1E-17	0.
CHCl3	1.8E-32	1.6E-31	4.0E-26	8.6E-39	1.2E-30	6.6E-26	0.
CCL4	0.	0.	3.8E-36	0.	0.	5.2E-36	0.
COCl2	6.4E-25	2.9E-24	1.3E-20	4.9E-34	5.2E-24	9.4E-21	2.0E-25
S2	1.1E-16	1.8E-16	5.5E-14	1.7E-21	2.7E-16	1.3E-13	0.
S8	0.	0.	1.5E-31	0.	0.	4.6E-30	0.
H2S	3.1E-04	3.4E-04	1.2E-04	3.4E-04	4.5E-04	3.1E-04	0.
SO2	1.4E-15	5.6E-16	3.7E-18	1.6E-23	6.3E-17	2.2E-18	3.5E-10
S03	2.4E-30	5.4E-31	6.9E-35	0.	1.8E-32	2.5E-35	2.5E-04
COS	4.6E-08	1.9E-07	2.5E-04	3.3E-17	2.6E-07	2.3E-04	0.
CS2	1.8E-15	1.7E-14	2.0E-08	2.8E-24	9.1E-14	4.4E-08	0.
SO	1.1E-22	7.7E-23	2.6E-23	7.1E-28	2.8E-23	2.5E-23	6.4E-38
SULFUROUS ACID	8.1E-35	1.5E-35	0.	0.	5.7E-37	0.	7.2E-30
SULFURIC ACID	9.1E-37	9.7E-38	0.	0.	0.	0.	3.4E-11
CYANOGENSULFIDE	3.6E-38	1.7E-36	5.1E-28	0.	3.8E-35	9.9E-28	0.
METHANEETHIOL	1.6E-10	8.8E-10	2.4E-08	5.4E-12	4.7E-09	1.0E-07	0.
DIMETHYLSULFIDE	1.7E-16	4.7E-15	1.0E-11	1.7E-19	9.9E-14	6.7E-11	0.
DIMET. DISULFIDE	9.1E-22	3.2E-20	1.2E-15	3.6E-27	8.3E-19	1.2E-14	0.
ETHANETHIOL	4.5E-15	1.3E-13	2.7E-10	4.7E-18	2.7E-12	1.8E-09	0.
DIETHYLSULFIDE	1.2E-25	8.6E-23	1.1E-15	1.2E-31	2.9E-20	1.9E-14	0.
DIETH. DISULFIDE	1.2E-30	1.1E-27	2.5E-19	0.	4.5E-25	6.5E-18	0.
ETHANECHITHIOL	1.2E-23	4.3E-22	1.6E-17	4.8E-29	1.1E-20	1.6E-16	0.
UCSTANETHIOL	0.	0.	2.5E-25	0.	4.3E-35	2.7E-23	0.
THIOFORMIC ACID	7.5E-25	2.7E-24	7.1E-23	1.5E-31	4.0E-24	1.1E-22	0.
THIOACETIC ACID	2.6E-27	4.7E-26	9.8E-23	1.6E-35	2.8E-25	2.4E-22	0.
CYCLOPROP.THIOL	6.9E-24	1.1E-21	9.5E-15	7.8E-31	8.8E-20	5.9E-14	0.
CYCLOBUTA.THIOL	1.7E-29	1.5E-26	9.5E-18	6.1E-38	4.5E-24	9.4E-17	0.
CYCLOPENT.THIOL	2.2E-30	9.4E-27	4.7E-16	0.	1.1E-23	7.5E-15	0.
CYCLOHEXA.THIOL	9.9E-33	2.2E-28	8.4E-16	0.	1.0E-24	2.1E-14	0.
M.SULFONIC ACID	5.3E-34	5.1E-34	1.0E-37	0.	7.5E-35	1.0E-37	0.
E.SULFINIC ACID	3.7E-11	5.8E-10	2.4E-08	6.5E-17	3.7E-09	9.9E-08	0.
THIOPHENE	1.9E-25	2.2E-22	3.5E-10	8.3E-39	5.6E-20	1.2E-09	0.
BENZENETHIOL	9.5E-32	3.3E-27	1.6E-09	0.	1.2E-23	8.1E-09	0.
THIICYANIC ACID	3.0E-21	2.2E-20	2.2E-16	4.5E-28	1.2E-19	4.9E-16	0.
THIOLGLYCOL	2.2E-29	3.5E-28	1.5E-26	3.9E-35	2.2E-27	6.0E-26	0.
CYSTEINE	1.3E-34	6.4E-33	3.0E-30	0.	5.4E-32	1.1E-29	0.
METHIONINE	0.	0.	4.2E-36	0.	0.	4.0E-35	0.

TABLE 22a

700°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-71.086	-22.007	-4.291	-8.848	-98.268	-11.895	-63.414
2	2.0	9.0	89.0	-70.963	-21.213	-4.334	-8.830	-98.152	-12.652	-63.258
3	2.0	19.0	79.0	-70.757	-20.774	-4.409	-8.802	-97.949	-13.037	-62.993
4	2.0	29.0	69.0	-70.497	-20.483	-4.511	-8.773	-97.682	-13.270	-62.656
5	2.0	39.0	59.0	-70.144	-20.231	-4.656	-8.742	-97.302	-13.460	-62.195
6	2.0	49.0	49.0	-69.594	-19.963	-4.898	-8.709	-96.681	-13.662	-61.476
7	2.0	59.0	39.0	-68.272	-19.522	-5.524	-8.674	-95.099	-14.033	-59.779
8	2.0	69.0	29.0	-6.579	-4.936	-34.923	-8.703	-38.521	-28.679	-16.490
9	2.0	79.0	19.0	-6.953	-4.528	-36.361	-8.767	-36.396	-29.209	-17.433
10	2.0	89.0	9.0	-4.595	-4.351	-37.792	-8.824	-34.278	-29.502	-17.901
11	2.0	96.0	2.0	0.501	-4.280	-42.185	-8.858	-27.705	-29.642	-18.110
12	10.0	2.0	88.0	-69.170	-21.909	-4.401	-8.805	-97.972	-11.908	-63.022
13	10.0	10.0	80.0	-68.973	-21.041	-4.477	-8.782	-97.771	-12.729	-62.766
14	10.0	20.0	70.0	-68.654	-20.600	-4.606	-8.752	-97.433	-13.110	-62.351
15	10.0	30.0	60.0	-68.183	-20.263	-4.809	-8.719	-96.909	-13.382	-61.736
16	10.0	40.0	50.0	-67.264	-19.872	-5.234	-8.685	-95.829	-13.705	-60.543
17	10.0	50.0	40.0	-8.856	-5.258	-34.451	-8.683	-39.219	-28.318	-15.807
18	10.0	60.0	30.0	-5.280	-4.645	-36.375	-8.750	-36.365	-29.063	-17.166
19	10.0	70.0	20.0	-2.865	-4.451	-37.848	-8.808	-34.186	-29.374	-17.671
20	10.0	80.0	10.0	1.806	-4.374	-41.845	-8.854	-28.214	-29.539	-17.916
21	10.0	88.0	2.0	5.381	-4.412	-46.717	-8.723	-20.840	-29.240	-17.578
22	20.0	2.0	78.0	-67.883	-21.730	-4.639	-8.745	-97.348	-11.967	-62.249
23	20.0	10.0	70.0	-67.490	-20.813	-4.809	-8.719	-96.909	-12.833	-61.736
24	20.0	20.0	60.0	-66.571	-20.219	-5.234	-8.685	-95.829	-13.358	-60.543
25	20.0	30.0	50.0	-7.182	-5.322	-34.950	-8.683	-38.470	-28.251	-15.678
26	20.0	40.0	40.0	-3.462	-4.750	-37.000	-8.750	-35.429	-28.960	-16.956
27	20.0	50.0	30.0	-1.262	-4.590	-38.461	-8.808	-33.267	-29.236	-17.392
28	20.0	60.0	20.0	2.698	-4.522	-42.023	-8.851	-27.945	-29.391	-17.615
29	20.0	70.0	10.0	6.773	-4.684	-46.411	-8.682	-21.278	-28.888	-16.951
30	22.0	76.0	2.0	8.050	-4.825	-48.938	-9.313	-17.804	-30.006	-17.931
31	18.0	80.0	2.0	7.923	-4.795	-48.898	-8.543	-17.478	-28.491	-16.453
32	30.0	2.0	68.0	-65.807	-21.279	-5.406	-8.678	-95.395	-12.283	-60.086
33	30.0	10.0	60.0	-5.188	-5.614	-35.770	-8.682	-37.240	-27.959	-15.092
34	30.0	20.0	50.0	-2.005	-5.035	-37.623	-8.749	-34.494	-28.669	-16.384
35	30.0	30.0	40.0	-0.261	-4.833	-38.899	-8.808	-32.610	-28.989	-16.906
36	30.0	40.0	30.0	3.494	-4.732	-42.400	-8.852	-27.380	-29.178	-17.242
37	30.0	50.0	20.0	8.092	-5.057	-47.066	-8.697	-20.304	-28.542	-16.315
38	30.0	60.0	10.0	8.143	-4.960	-47.541	-8.562	-19.524	-28.369	-16.204
39	30.0	68.0	2.0	8.122	-4.853	-48.849	-8.419	-17.491	-28.188	-16.088
40	40.0	10.0	50.0	0.435	-5.376	-39.219	-8.808	-32.131	-28.443	-15.995
41	40.0	20.0	40.0	4.491	-5.088	-43.101	-8.855	-26.330	-28.826	-16.610
42	40.0	30.0	30.0	8.292	-5.306	-46.950	-8.742	-20.501	-28.383	-16.001
43	40.0	40.0	20.0	8.275	-5.179	-47.104	-8.624	-20.210	-28.275	-15.986
44	40.0	50.0	10.0	8.232	-5.035	-47.443	-8.469	-19.624	-28.107	-15.823
45	40.0	58.0	2.0	8.183	-4.893	-48.657	-8.292	-17.715	-27.895	-15.754

TABLE 22b

700°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	4.7E-09	7.9E-06	1.4E-04	6.9E-03	2.9E-01	3.7E-01	0.
H2	1.4E-01	3.7E-01	3.2E-01	7.9E-01	4.3E-01	2.5E-01	6.4E-15
O2	6.0E-27	3.6E-29	8.2E-31	2.3E-33	2.4E-37	2.5E-38	5.0E-01
WATER	5.8E-01	1.2E-01	1.6E-02	2.1E-03	1.2E-05	2.2E-06	2.5E-01
CO	7.3E-03	1.3E-01	4.6E-01	1.9E-01	2.9E-01	3.6E-01	7.1E-16
CO2	2.8E-01	3.7E-01	2.1E-01	4.5E-03	7.0E-05	2.9E-05	2.5E-01
BENZENE	0.	1.8E-33	2.3E-25	8.9E-19	1.2E-06	8.6E-04	0.
NAPHTHALENE	0.	0.	0.	9.9E-30	3.1E-09	3.0E-04	0.
ASPHALT	0.	0.	0.	0.	3.5E-14	1.6E-02	0.
ACETYLENE	3.5E-23	4.7E-18	2.4E-15	3.7E-13	4.1E-09	3.7E-08	0.
ETHYLENE	6.2E-21	2.3E-15	9.8E-13	3.9E-10	2.3E-06	1.2E-05	0.
ETHANE	8.0E-22	8.1E-16	3.0E-13	2.9E-10	9.4E-07	2.8E-06	0.
FORMIC ACID	3.4E-12	1.3E-11	6.0E-12	3.3E-13	2.7E-15	6.4E-16	1.5E-25
ACETIC ACID	7.3E-21	1.7E-17	1.6E-16	1.7E-16	1.1E-16	6.0E-17	0.
FORMALDEHYDE	4.9E-13	2.3E-11	7.2E-11	7.5E-11	6.0E-11	4.4E-11	0.
ACETALDEHYDE	1.2E-22	3.3E-18	2.2E-16	4.4E-15	2.8E-13	4.6E-13	0.
METHANOL	4.1E-17	5.3E-15	1.4E-14	3.7E-14	1.6E-14	6.7E-15	0.
ETHANOL	2.9E-28	2.3E-23	1.3E-21	6.6E-20	2.2E-18	2.1E-18	0.
N2	1.4E-04	1.3E-04	1.1E-04	1.0E-04	1.4E-04	1.8E-04	1.3E-04
NH3	1.1E-09	4.8E-09	3.5E-09	1.3E-08	6.2E-09	3.1E-09	1.1E-29
HCN	7.2E-15	2.5E-12	5.2E-11	6.3E-10	7.8E-08	2.6E-07	0.
NO	7.6E-22	5.5E-23	7.8E-24	3.9E-25	4.8E-27	1.8E-27	6.5E-09
NO2	1.8E-36	1.0E-38	0.	0.	0.	0.	1.4E-10
N2O	1.5E-29	1.0E-30	1.3E-31	6.5E-33	9.5E-35	3.9E-35	1.2E-16
NITROUS ACID	2.4E-33	2.3E-35	4.5E-37	0.	0.	0.	4.1E-14
NITRIC ACID	0.	0.	0.	0.	0.	0.	1.8E-16
C2N2	3.4E-33	1.4E-28	7.7E-26	4.4E-24	1.3E-19	2.5E-18	0.
HNCO	6.9E-15	1.8E-13	5.9E-13	3.7E-13	4.8E-13	5.2E-13	1.4E-34
P2	4.3E-31	8.4E-28	2.4E-25	1.6E-21	1.6E-15	5.5E-14	0.
P4O6	7.2E-05	6.3E-05	5.6E-05	5.1E-05	7.2E-05	9.2E-05	3.2E-28
P4O10	2.1E-33	6.7E-38	0.	0.	0.	0.	6.3E-05
PO	2.6E-21	9.0E-21	2.2E-20	9.6E-20	1.0E-18	1.9E-18	1.2E-33
PO2	2.5E-18	6.8E-19	2.6E-19	5.7E-20	6.4E-21	3.8E-21	1.1E-17
PH2	2.7E-19	3.3E-17	4.7E-16	9.7E-14	5.3E-11	1.8E-10	0.
PH3	3.6E-21	7.4E-19	9.6E-18	3.1E-15	1.3E-12	3.2E-12	0.
PCL3	1.5E-31	9.8E-31	1.5E-29	2.3E-28	1.7E-24	4.6E-23	5.1E-37
POCL3	3.4E-30	1.7E-30	4.0E-30	3.2E-30	2.4E-28	2.2E-27	1.1E-22
PSCL3	1.3E-30	2.7E-30	4.4E-29	2.5E-28	4.8E-24	2.8E-22	0.
CL2	1.3E-21	3.5E-22	3.3E-22	1.1E-22	4.0E-22	1.1E-21	2.0E-08
HCl	2.9E-04	2.5E-04	2.3E-04	2.1E-04	2.9E-04	3.7E-04	2.5E-04
HOCl	4.9E-22	3.4E-23	4.5E-24	2.2E-25	3.1E-27	1.3E-27	3.9E-09
Cl2O	0.	0.	0.	0.	0.	0.	3.5E-19
CH3Cl	4.3E-18	2.3E-15	4.3E-14	7.7E-13	8.4E-11	2.4E-10	0.
CH2Cl2	6.3E-28	1.1E-25	2.1E-24	1.4E-23	3.9E-21	2.5E-20	0.
CHCl3	4.7E-38	2.5E-36	5.2E-35	1.3E-34	9.3E-32	1.3E-30	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
COCl2	1.8E-26	8.8E-26	3.0E-25	4.2E-26	2.3E-25	8.3E-25	2.9E-26
S2	9.3E-11	9.4E-12	1.0E-11	1.4E-12	9.4E-12	4.2E-11	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	2.9E-04	2.5E-04	2.3E-04	2.1E-04	2.9E-04	3.5E-04	8.4E-38
SO2	1.3E-10	2.6E-13	6.1E-15	6.1E-18	1.7E-21	3.8E-22	6.8E-05
SO3	4.0E-23	6.0E-27	2.1E-29	1.1E-33	0.	0.	1.9E-04
COS	4.8E-07	2.6E-06	1.0E-05	1.5E-06	6.0E-06	1.6E-05	0.
CS2	1.9E-13	4.1E-12	1.1E-10	1.2E-10	1.2E-07	2.0E-06	0.
SO	6.2E-14	1.5E-15	2.4E-16	4.7E-18	1.3E-19	8.7E-20	3.5E-21
SULFUROUS ACID	5.8E-31	2.4E-34	7.2E-37	0.	0.	0.	1.3E-25
SULFURIC ACID	4.1E-34	1.3E-38	0.	0.	0.	0.	8.3E-16
CYANOGENSULFIDE	1.3E-37	1.8E-33	1.0E-30	2.1E-29	1.6E-24	6.7E-23	0.
METHANETHIOL	2.5E-17	1.3E-14	2.4E-13	4.4E-12	4.0E-10	1.3E-09	0.
DIMETHYLSULFIDE	2.5E-30	8.0E-25	3.1E-22	1.1E-19	9.2E-16	5.8E-15	0.
DIMET.CISULFIDE	1.3E-36	1.3E-31	5.3E-29	6.9E-27	1.5E-22	2.0E-21	0.
ETHANETHIOL	3.7E-29	1.2E-23	4.6E-21	1.6E-18	1.4E-14	8.7E-14	0.
DIETHYLSULFIDE	0.	0.	9.8E-38	1.4E-32	6.9E-25	2.2E-23	0.
DIETH.DISULFIDE	0.	0.	0.	0.	1.7E-31	1.1E-29	0.
ETHANEDIITHIOL	1.1E-37	1.1E-32	4.6E-30	6.0E-28	1.3E-23	1.7E-22	0.
OCTANETHIOL	0.	0.	0.	0.	0.	0.	0.
THIOFCRMIC ACID	9.6E-24	1.4E-22	4.7E-22	1.8E-22	3.8E-22	5.8E-22	0.
THIUACETIC ACID	9.2E-35	8.4E-31	5.7E-29	4.3E-28	7.0E-26	2.5E-25	0.
CYCLOPRCP.THICL	1.2E-37	8.3E-30	7.8E-26	2.2E-22	2.7E-16	6.6E-15	0.
CYCLOBUTA.THICL	0.	0.	1.5E-34	8.6E-30	8.0E-22	4.4E-20	0.
CYCLOPENT.THICL	0.	0.	0.	2.7E-35	2.0E-25	2.5E-23	0.
CYCLO-EXA.THOL	0.	0.	0.	4.2E-39	2.3E-27	6.6E-25	0.
M.SULFINIC ACID	0.	0.	0.	0.	0.	0.	0.
E.SULFINIC ACID	1.5E-29	3.9E-25	2.2E-23	4.2E-22	3.7E-20	7.4E-20	0.
THIOPHENNE	8.6E-39	4.9E-29	1.3E-23	1.2E-19	3.8E-11	6.5E-09	0.
BENZENETHIOL	0.	0.	2.5E-32	3.5E-26	1.3E-13	1.9E-10	0.
THIOCYANIC ACID	7.9E-21	8.6E-19	1.9E-17	8.4E-17	2.8E-14	2.0E-13	0.
THIOLGLYCOL	0.	6.9E-37	4.0E-35	7.4E-34	6.5E-32	1.3E-31	0.
CYSTEINE	0.	0.	0.	0.	0.	0.	0.
METHICININE	0.	0.	0.	0.	0.	0.	0.

TABLE 23a

700°K AND 0.2 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MCLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-71.086	-20.280	-0.837	-5.394	-105.176	-6.717	-66.633
2	2.0	9.0	89.0	-70.963	-19.486	-0.880	-5.376	-105.060	-7.474	-66.468
3	2.0	19.0	79.0	-70.757	-19.047	-0.956	-5.348	-104.857	-7.864	-66.185
4	2.0	29.0	69.0	-70.497	-18.756	-1.057	-5.319	-104.590	-8.091	-65.824
5	2.0	39.0	59.0	-70.144	-18.504	-1.202	-5.288	-104.210	-8.281	-65.326
6	2.0	49.0	49.0	-69.594	-18.236	-1.444	-5.255	-103.588	-8.483	-64.534
7	2.0	59.0	39.0	-68.271	-17.795	-2.070	-5.220	-102.006	-8.854	-62.585
8	2.0	69.0	29.0	-2.957	-1.519	-34.824	-5.244	-36.940	-25.176	-16.408
9	2.0	79.0	19.0	-2.307	-1.177	-35.908	-5.289	-35.329	-25.580	-17.156
10	2.0	89.0	9.0	-3.057	-0.954	-37.163	-5.354	-33.472	-25.908	-17.706
11	2.0	96.0	2.0	-3.538	-0.850	-38.954	-5.405	-30.805	-26.090	-17.991
12	10.0	2.0	88.0	-69.170	-20.182	-0.947	-5.351	-104.880	-6.729	-66.217
13	10.0	10.0	80.0	-68.973	-19.314	-1.023	-5.328	-104.679	-7.551	-65.943
14	10.0	20.0	70.0	-68.654	-18.873	-1.152	-5.298	-104.341	-7.931	-65.495
15	10.0	30.0	60.0	-68.183	-18.536	-1.355	-5.266	-103.817	-8.203	-64.822
16	10.0	40.0	50.0	-67.264	-18.145	-1.780	-5.231	-102.737	-8.525	-63.477
17	10.0	50.0	40.0	-2.156	-1.847	-34.349	-5.227	-37.643	-24.809	-15.717
18	10.0	60.0	30.0	-0.479	-1.477	-35.353	-5.230	-36.137	-25.180	-16.455
19	10.0	70.0	20.0	-0.126	-1.353	-35.815	-5.210	-35.432	-25.259	-16.660
20	10.0	80.0	10.0	-0.218	-1.217	-36.467	-5.197	-34.447	-25.360	-16.897
21	10.0	88.0	2.0	-0.945	-1.021	-38.329	-5.235	-31.668	-25.613	-17.346
22	20.0	2.0	78.0	-67.883	-20.004	-1.185	-5.291	-104.256	-6.788	-65.385
23	20.0	10.0	70.0	-67.490	-19.086	-1.355	-5.266	-103.817	-7.662	-64.822
24	20.0	20.0	60.0	-66.571	-18.492	-1.780	-5.231	-102.737	-8.179	-63.477
25	20.0	30.0	50.0	-0.782	-1.975	-34.690	-5.222	-37.129	-24.673	-15.451
26	20.0	40.0	40.0	0.734	-1.710	-35.537	-5.206	-35.850	-24.904	-15.947
27	20.0	50.0	30.0	1.345	-1.659	-35.949	-5.170	-35.215	-24.881	-15.975
28	20.0	60.0	20.0	1.894	-1.663	-36.381	-5.123	-34.542	-24.784	-15.874
29	20.0	70.0	10.0	2.640	-1.740	-37.060	-5.064	-33.495	-24.589	-15.602
30	22.0	76.0	2.0	7.185	-2.778	-41.108	-5.783	-27.783	-24.991	-15.097
31	18.0	80.0	2.0	2.225	-1.587	-37.866	-5.035	-32.271	-24.682	-15.850
32	30.0	2.0	68.0	-65.806	-19.552	-1.952	-5.224	-102.302	-7.105	-62.946
33	30.0	10.0	60.0	1.032	-2.336	-35.407	-5.218	-36.051	-24.304	-14.721
34	30.0	20.0	50.0	2.878	-2.233	-36.421	-5.200	-34.522	-24.368	-14.892
35	30.0	30.0	40.0	4.259	-2.405	-37.246	-5.178	-33.273	-24.153	-14.659
36	30.0	40.0	30.0	5.716	-2.672	-38.232	-5.165	-31.788	-23.860	-14.320
37	30.0	50.0	20.0	7.273	-2.990	-39.526	-5.141	-29.836	-23.493	-14.011
38	30.0	60.0	10.0	7.336	-2.916	-39.936	-5.025	-29.162	-23.335	-13.696
39	30.0	68.0	2.0	7.325	-2.826	-41.096	-4.893	-27.356	-23.161	-13.254
40	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
41	40.0	20.0	40.0	7.510	-3.360	-39.372	-5.266	-30.129	-23.373	-14.267
42	40.0	30.0	30.0	7.508	-3.239	-39.456	-5.179	-29.960	-23.321	-14.092
43	40.0	40.0	20.0	7.477	-3.119	-39.577	-5.072	-29.725	-23.226	-13.854
44	40.0	50.0	10.0	7.437	-2.992	-39.869	-4.933	-29.217	-23.074	-13.501
45	40.0	58.0	2.0	7.395	-2.870	-40.938	-4.771	-27.533	-22.872	-12.976

TABLE 23B

700°K AND 0.2 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.2E-03	1.0E-01	2.1E-01	2.8E-01	6.0E-01	5.9E-01	0.
H2	1.2E-01	1.6E-01	4.1E-02	4.4E-01	1.5E-01	1.5E-02	2.0E-16
O2	7.3E-30	6.8E-31	2.2E-32	1.1E-31	3.2E-32	1.0E-34	5.0E-01
WATER	5.9E-01	2.4E-01	1.1E-02	2.5E-01	4.8E-02	2.6E-04	2.5E-01
CO	6.6E-03	3.6E-02	2.2E-01	5.5E-03	5.3E-02	3.3E-01	2.3E-17
CO2	2.8E-01	4.6E-01	5.2E-01	2.8E-02	1.5E-01	5.2E-02	2.5E-01
BENZENE	1.6E-25	1.3E-17	3.0E-10	8.0E-19	9.7E-13	1.4E-03	0.
NAPHTHALENE	0.	3.9E-28	3.1E-15	1.5E-30	5.8E-20	1.2E-03	0.
ASPHALT	0.	0.	2.6E-29	0.	0.	1.4E-02	0.
ACETYLENE	2.1E-17	9.0E-15	2.6E-12	3.6E-15	3.8E-13	4.4E-10	0.
ETHYLENE	3.4E-12	1.9E-09	1.4E-07	2.1E-09	7.7E-08	8.3E-06	0.
ETHANE	4.1E-10	3.0E-07	5.4E-06	8.6E-07	1.1E-05	1.2E-04	0.
FORMIC ACID	3.2E-09	6.9E-09	1.9E-09	1.1E-09	2.1E-09	6.9E-11	4.6E-24
ACETIC ACID	5.0E-12	2.6E-10	6.1E-10	4.3E-11	5.0E-10	1.7E-10	0.
FORMALDEHYDE	4.0E-10	2.9E-09	4.4E-09	1.2E-09	4.0E-09	2.3E-09	0.
ACETALDEHYDE	7.1E-14	1.2E-11	1.6E-10	5.1E-12	1.1E-10	6.5E-10	0.
METHANOL	3.1E-11	2.9E-10	1.1E-10	3.2E-10	3.8E-10	2.1E-11	0.
ETHANOL	1.6E-16	3.7E-14	1.2E-13	4.2E-14	3.0E-13	1.8E-13	0.
N2	1.4E-04	1.5E-04	1.6E-04	1.5E-04	2.0E-04	2.2E-04	1.3E-04
NH3	9.7E-07	1.5E-06	1.9E-07	6.7E-06	1.6E-06	4.8E-08	6.0E-29
HCN	5.6E-12	1.2E-10	2.1E-09	7.5E-11	8.9E-10	3.1E-08	0.
NO	2.7E-23	8.3E-24	1.5E-24	3.3E-24	2.1E-24	1.2E-25	6.5E-09
NO2	7.0E-38	6.6E-39	0.	0.	0.	0.	4.4E-09
N2O	1.6E-29	5.2E-30	1.0E-30	2.1E-30	1.5E-30	9.2E-32	3.7E-15
NITROUS ACID	2.9E-33	3.1E-34	5.2E-36	8.0E-35	1.7E-35	1.7E-38	7.4E-12
NITRIC ACID	0.	0.	0.	0.	0.	0.	9.9E-13
C2N2	2.3E-27	7.6E-25	9.3E-22	1.2E-25	4.6E-23	5.9E-19	0.
HNC0	6.0E-12	3.8E-11	1.2E-10	9.6E-12	6.3E-11	1.2E-10	7.7E-34
P2	1.0E-32	3.6E-31	6.3E-29	6.0E-30	4.0E-29	2.3E-25	0.
P406	7.3E-05	7.6E-05	8.0E-05	7.9E-05	1.0E-04	1.1E-04	3.2E-34
P4010	3.1E-33	2.8E-35	3.2E-38	7.1E-37	8.4E-38	0.	6.3E-05
PO	1.4E-23	2.5E-23	6.0E-23	4.1E-23	5.8E-23	2.5E-22	3.9E-38
PO2	1.5E-20	8.3E-21	3.6E-21	5.3E-21	4.2E-21	1.0E-21	1.1E-20
PH2	1.2E-18	9.6E-18	3.1E-17	1.0E-16	9.5E-17	6.9E-16	0.
PH3	4.9E-19	4.4E-18	7.2E-18	7.9E-17	4.3E-17	9.5E-17	0.
PCL3	2.7E-29	1.2E-28	1.5E-26	1.3E-28	3.3E-27	1.1E-23	2.9E-36
POCL3	6.8E-28	9.4E-28	2.1E-26	3.8E-28	5.6E-27	1.0E-24	1.9E-20
PSCL3	2.6E-28	9.5E-28	4.3E-25	3.8E-28	3.6E-26	8.0E-22	0.
CL2	1.4E-21	1.2E-21	5.2E-21	4.7E-22	2.2E-21	2.7E-20	6.5E-07
HCL	2.9E-04	3.0E-04	3.2E-04	3.2E-04	4.0E-04	4.4E-04	2.5E-04
HOCL	5.5E-22	1.7E-22	3.3E-23	7.2E-23	5.1E-23	3.1E-24	1.2E-07
CL20	0.	0.	0.	0.	0.	0.	3.5E-16
CH3CL	3.3E-12	8.0E-11	7.2E-10	8.6E-11	6.8E-10	7.6E-09	0.
CH2CL2	5.2E-22	1.0E-20	3.9E-19	4.2E-21	1.2E-19	1.6E-17	0.
CHCL3	4.4E-32	6.8E-31	1.1E-28	1.1E-31	1.1E-29	1.7E-26	0.
CCL4	0.	0.	0.	0.	0.	1.5E-36	0.
COCL2	1.9E-23	8.4E-23	2.3E-21	5.1E-24	2.3E-22	1.8E-20	2.9E-23
S2	1.1E-13	7.0E-14	9.3E-13	1.1E-14	1.4E-13	6.3E-12	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	2.9E-04	3.0E-04	2.7E-04	3.2E-04	4.0E-04	2.6E-04	0.
SO2	1.8E-13	1.3E-14	1.6E-15	7.9E-16	8.8E-16	1.9E-17	2.9E-06
SO3	5.9E-26	1.3E-27	2.9E-29	3.2E-29	2.0E-29	2.3E-32	2.5E-04
COS	4.7E-07	2.1E-06	4.6E-05	1.2E-07	4.3E-06	1.8E-04	0.
CS2	1.8E-13	2.1E-12	9.2E-10	1.2E-13	2.8E-11	1.4E-07	0.
SO	7.6E-17	1.8E-17	1.2E-17	2.8E-18	5.6E-18	2.1E-18	4.8E-24
SULFURIC ACID	7.9E-31	2.3E-32	1.3E-34	1.5E-33	3.2E-34	3.7E-38	5.5E-24
SULFURIC ACID	6.2E-34	5.6E-36	5.4E-39	1.4E-37	1.7E-38	0.	1.1E-12
CYANOGENSULFIDE	9.7E-32	2.6E-29	1.1E-25	1.5E-30	2.2E-27	1.9E-22	0.
METHANETHIOL	1.8E-11	4.6E-10	3.5E-09	4.9E-10	3.8E-09	2.6E-08	0.
DIMETHYLSULFIDE	1.4E-18	8.0E-16	5.2E-14	8.9E-16	4.3E-14	3.0E-12	0.
DIMET.CISULFIDE	7.8E-25	3.6E-22	8.5E-20	1.5E-22	2.7E-20	1.3E-17	0.
ETHANETHIOL	2.1E-17	1.2E-14	7.8E-13	1.3E-14	6.4E-13	4.5E-11	0.
DIETHYLSULFIDE	1.5E-30	5.0E-25	2.3E-21	5.9E-25	1.1E-21	8.0E-18	0.
DIETH.DISULFIDE	1.3E-36	3.3E-31	5.5E-27	1.5E-31	9.9E-28	5.0E-23	0.
ETHANECHITILL	6.8E-26	3.2E-23	7.4E-21	1.4E-23	2.4E-21	1.1E-18	0.
OCTANECHITILL	0.	0.	3.0E-37	0.	4.2E-38	3.8E-30	0.
THIOFORMIC ACID	8.7E-21	5.0E-20	2.8E-19	7.9E-21	9.7E-20	3.8E-19	0.
THIOACETIC ACID	6.2E-26	8.4E-24	4.0E-22	1.4E-24	1.0E-22	4.3E-21	0.
CYCLOPRCP.THICL	5.3E-23	5.6E-19	1.2E-15	2.4E-19	2.0E-16	1.5E-12	0.
CYCLOBUTA.THIOL	6.1E-30	1.5E-24	2.8E-20	6.7E-25	3.4E-21	2.7E-16	0.
CYCLOPENT.THIOL	5.8E-35	3.4E-28	5.4E-23	1.6E-28	4.9E-24	4.1E-18	0.
CYCLOHEXA.THIOL	2.6E-38	3.7E-30	4.9E-24	1.7E-30	3.3E-25	2.9E-18	0.
M-SULFCNIC ACID	2.5E-33	1.7E-33	7.9E-35	1.1E-34	1.5E-34	1.8E-37	0.
E-SULFINIC ACID	9.5E-18	1.7E-15	2.0E-14	7.4E-16	2.0E-14	7.7E-14	0.
THIOPHENNE	3.5E-24	5.0E-19	1.5E-13	3.1E-20	1.3E-15	1.1E-08	0.
BENZENETHIOL	5.8E-32	3.6E-24	3.1E-16	8.8E-26	3.9E-19	3.9E-09	0.
THIOCYANIC ACID	6.8E-18	1.1E-16	7.2E-15	2.0E-17	1.2E-15	2.8E-13	0.
THIOGLYCOL	1.7E-29	3.0E-27	3.5E-26	1.3E-27	3.5E-26	1.4E-25	0.
CYSTEINE	7.8E-39	9.0E-36	3.3E-34	9.9E-37	1.7E-34	1.3E-33	0.
METHICNINE	0.	0.	0.	0.	0.	0.	0.

TABLE 24a

700°K AND 20 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\bar{F}_i/RT$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-71.086	-19.128	1.466	-3.092	-109.782	-3.656	-68.940
2	2.0	9.0	89.0	-70.963	-18.335	1.423	-3.073	-109.665	-4.148	-68.775
3	2.0	19.0	79.0	-70.757	-17.896	1.347	-3.046	-109.462	-4.409	-68.493
4	2.0	29.0	69.0	-70.497	-17.605	1.246	-3.017	-109.195	-4.642	-68.132
5	2.0	39.0	59.0	-70.144	-17.353	1.100	-2.986	-108.815	-4.831	-67.633
6	2.0	49.0	49.0	-69.594	-17.085	0.858	-2.953	-108.194	-5.044	-66.841
7	2.0	59.0	39.0	-68.271	-16.644	0.232	-2.918	-106.611	-5.398	-64.893
8	2.0	69.0	29.0	-2.949	0.204	-33.461	-2.974	-37.811	-22.203	-15.161
9	2.0	79.0	19.0	-6.476	1.087	-35.760	-3.956	-34.394	-23.215	-17.051
10	2.0	89.0	9.0	-7.645	1.348	-37.155	-4.717	-32.333	-23.602	-17.701
11	2.0	96.0	2.0	-8.142	1.452	-38.953	-5.109	-29.656	-23.786	-17.989
12	10.0	2.0	88.0	-69.170	-19.030	1.356	-3.048	-109.485	-3.642	-68.524
13	10.0	10.0	80.0	-68.973	-18.163	1.280	-3.026	-109.284	-4.201	-68.251
14	10.0	20.0	70.0	-68.654	-17.721	1.151	-2.995	-108.946	-4.482	-67.803
15	10.0	30.0	60.0	-68.183	-17.385	0.948	-2.963	-108.422	-4.753	-67.130
16	10.0	40.0	50.0	-67.264	-16.994	0.522	-2.928	-107.342	-5.071	-65.785
17	10.0	50.0	40.0	-1.156	-0.373	-32.558	-2.909	-39.164	-21.624	-14.004
18	10.0	60.0	30.0	-0.538	-0.133	-33.094	-2.886	-38.342	-21.790	-14.410
19	10.0	70.0	20.0	-0.683	0.066	-33.566	-2.868	-37.615	-21.912	-14.732
20	10.0	80.0	10.0	-4.089	0.948	-35.902	-3.492	-34.125	-22.852	-16.552
21	10.0	88.0	2.0	-5.541	1.280	-38.306	-4.289	-30.550	-23.308	-17.340
22	20.0	2.0	78.0	-67.883	-18.852	1.118	-2.989	-108.861	-3.648	-67.692
23	20.0	10.0	70.0	-67.490	-17.934	0.948	-2.963	-108.422	-4.203	-67.130
24	20.0	20.0	60.0	-66.571	-17.341	0.522	-2.928	-107.342	-4.727	-65.785
25	20.0	30.0	50.0	-0.167	-0.605	-32.678	-2.900	-38.983	-21.386	-13.535
26	20.0	40.0	40.0	0.691	-0.433	-33.179	-2.866	-38.213	-21.477	-13.801
27	20.0	50.0	30.0	1.134	-0.378	-33.501	-2.824	-37.708	-21.449	-13.824
28	20.0	60.0	20.0	1.536	-0.364	-33.856	-2.777	-37.152	-21.367	-13.757
29	20.0	70.0	10.0	2.058	-0.401	-34.408	-2.722	-36.298	-21.224	-13.578
30	22.0	76.0	2.0	6.709	-1.495	-37.457	-3.458	-32.097	-21.620	-13.103
31	18.0	80.0	2.0	-0.640	0.310	-35.944	-2.781	-33.985	-21.900	-14.966
32	30.0	2.0	68.0	-65.806	-18.400	0.350	-2.921	-106.907	-3.829	-65.254
33	30.0	10.0	60.0	1.643	-1.050	-33.372	-2.894	-37.941	-20.934	-12.638
34	30.0	20.0	50.0	4.253	-1.327	-34.721	-2.657	-35.901	-20.589	-12.019
35	30.0	30.0	40.0	6.882	-1.864	-36.140	-2.827	-33.758	-19.991	-12.092
36	30.0	40.0	30.0	6.896	-1.778	-36.239	-2.771	-33.581	-19.966	-11.982
37	30.0	50.0	20.0	6.880	-1.693	-36.376	-2.708	-33.344	-19.924	-11.823
38	30.0	60.0	10.0	6.857	-1.609	-36.651	-2.634	-32.895	-19.861	-11.606
39	30.0	68.0	2.0	6.836	-1.540	-37.438	-2.564	-31.678	-19.789	-11.280
40	40.0	10.0	50.0	7.351	-2.530	-36.258	-2.819	-33.576	-19.306	-12.075
41	40.0	20.0	40.0	7.152	-2.135	-36.207	-2.758	-33.622	-19.583	-11.988
42	40.0	30.0	30.0	7.061	-1.943	-36.241	-2.691	-33.538	-19.640	-11.831
43	40.0	40.0	20.0	6.998	-1.801	-36.340	-2.615	-33.352	-19.630	-11.648
44	40.0	50.0	10.0	6.945	-1.678	-36.581	-2.525	-32.944	-19.572	-11.394
45	40.0	58.0	2.0	6.905	-1.581	-37.334	-2.436	-31.770	-19.491	-11.011

TABLE 24b

700°K AND 20 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.2E-02	1.6E-01	2.5E-01	3.3E-01	7.1E-01	6.8E-01	0.
H2	2.4E-02	2.1E-02	1.2E-03	3.3E-01	2.2E-02	2.0E-03	2.0E-17
U2	2.6E-30	7.6E-31	2.0E-33	3.3E-33	6.5E-32	7.3E-34	5.0E-01
WATER	6.7E-01	3.2E-01	9.5E-04	3.3E-01	1.0E-01	9.5E-04	2.5E-01
CO	1.1E-03	3.6E-03	9.2E-02	2.0E-06	4.2E-03	5.4E-02	2.3E-18
CO2	2.7E-01	5.0E-01	6.5E-01	1.8E-05	1.7E-01	2.3E-01	2.5E-01
BENZENE	4.5E-21	2.1E-16	5.2E-04	2.9E-25	9.1E-13	2.1E-03	0.
NAPHTHALENE	1.1E-33	7.0E-26	5.7E-04	0.	7.8E-20	3.4E-03	0.
ASPHALT	0.	0.	1.9E-03	0.	0.	2.4E-02	0.
ACETYLENE	3.0E-17	1.1E-15	1.4E-11	1.2E-18	1.7E-14	2.3E-11	0.
ETHYLENE	9.2E-11	2.9E-09	2.3E-06	5.1E-11	5.1E-08	6.0E-06	0.
ETHANE	2.1E-07	5.8E-06	2.6E-04	1.6E-06	1.1E-04	1.1E-03	0.
FORMIC ACID	5.9E-08	9.5E-08	7.1E-09	5.5E-11	3.4E-08	4.2E-09	4.6E-23
ACETIC ACID	4.8E-09	4.4E-08	9.2E-08	3.4E-12	6.6E-08	8.7E-08	0.
FORMALDEHYDE	1.2E-09	3.8E-09	5.4E-09	3.3E-11	4.6E-09	5.3E-09	0.
ACETALDEHYCE	1.1E-11	1.9E-10	7.8E-09	2.3E-13	9.9E-10	1.2E-08	0.
METHANOL	1.8E-09	4.9E-09	4.0E-10	6.8E-10	6.4E-09	6.6E-10	0.
ETHANOL	5.0E-13	7.6E-12	1.7E-11	1.4E-13	4.1E-11	4.6E-11	0.
N2	1.5E-04	1.6E-04	1.8E-04	4.6E-05	2.2E-04	2.6E-04	1.3E-04
NH3	8.3E-06	7.2E-06	1.0E-07	2.4E-04	9.1E-06	2.7E-07	1.9E-28
HCN	6.7E-12	4.2E-11	5.1E-09	7.5E-13	2.0E-10	7.8E-09	0.
NO	1.6E-23	9.1E-24	4.9E-25	3.2E-25	3.1E-24	3.5E-25	6.5E-09
NO2	2.5E-37	7.7E-38	0.	0.	7.6E-39	0.	4.4E-08
N2O	1.0E-28	5.9E-29	3.3E-30	1.1E-30	2.3E-29	2.9E-30	3.7E-14
NITROUS ACID	4.6E-32	1.3E-32	8.6E-36	1.2E-34	1.3E-33	4.9E-36	2.3E-10
NITRIC ACID	0.	0.	0.	0.	0.	0.	3.1E-10
C2N2	1.7E-26	7.5E-25	1.9E-19	1.5E-29	1.5E-23	2.7E-19	0.
HNCO	4.3E-11	1.4E-10	9.1E-10	1.7E-13	2.0E-10	8.3E-10	2.4E-33
P2	4.8E-36	3.2E-35	2.4E-31	1.1E-31	1.5E-33	1.3E-30	0.
P4O6	7.7E-05	8.3E-05	8.8E-05	8.4E-05	1.1E-04	1.3E-04	3.2E-38
P4O10	4.3E-30	3.8E-31	2.9E-36	7.2E-36	3.8E-33	5.6E-37	6.3E-05
PO	1.8E-25	2.5E-25	1.1E-24	9.9E-25	5.0E-25	1.6E-24	0.
PO2	1.2E-21	8.8E-22	2.0E-22	2.3E-22	5.1E-22	1.7E-22	1.1E-22
PH2	5.1E-20	1.2E-19	5.7E-19	1.1E-16	8.4E-19	2.3E-18	0.
PH3	8.9E-20	1.9E-19	2.3E-19	7.2E-16	1.4E-18	1.1E-18	0.
PCl3	8.4E-28	3.4E-27	2.5E-23	3.3E-27	4.9E-26	8.8E-23	9.0E-36
POCl3	1.3E-25	2.7E-25	1.1E-22	1.7E-26	1.2E-24	2.2E-22	5.9E-19
PSCl3	4.5E-26	2.2E-25	9.1E-21	1.4E-26	4.0E-24	5.2E-20	0.
Cl2	8.3E-21	1.1E-20	2.2E-19	7.1E-22	1.8E-20	2.8E-19	6.4E-06
HCl	3.1E-04	3.4E-04	3.5E-04	3.4E-04	4.5E-04	5.2E-04	2.5E-04
HOCl	3.5E-21	2.0E-21	1.1E-22	1.3E-22	7.9E-22	9.8E-23	1.2E-06
Cl2O	0.	0.	0.	0.	0.	0.	3.5E-14
CH3Cl	1.8E-10	1.1E-09	3.2E-08	1.5E-10	6.1E-09	7.7E-08	0.
CH2Cl2	1.6E-19	1.2E-18	6.5E-16	1.0E-20	8.3E-18	1.4E-15	0.
CHCl3	7.3E-29	6.8E-28	6.8E-24	3.7E-31	5.9E-27	1.3E-23	0.
CCL4	0.	3.2E-38	5.9E-33	0.	3.5E-37	9.8E-33	8.2E-39
COCl2	1.8E-21	8.0E-21	4.0E-18	2.8E-25	1.5E-20	3.0E-18	2.9E-21
S2	3.4E-14	5.1E-14	1.6E-12	2.1E-16	8.0E-14	4.1E-12	0.
S8	0.	0.	8.1E-38	0.	0.	4.0E-36	0.
H2S	3.1E-04	3.3E-04	1.1E-04	3.4E-04	4.4E-04	2.9E-04	0.
SO2	3.6E-13	1.3E-13	1.9E-15	3.5E-17	1.3E-14	1.1E-15	2.9E-07
SO3	7.1E-25	1.3E-25	1.0E-28	2.4E-30	4.2E-27	3.6E-29	2.5E-04
COS	4.3E-07	1.8E-06	2.5E-04	6.3E-11	2.6E-06	2.4E-04	0.
CS2	1.5E-13	1.4E-12	2.2E-08	5.0E-17	8.9E-12	5.6E-08	0.
SO	2.5E-17	1.7E-17	4.7E-18	6.9E-20	6.0E-18	4.6E-18	4.7E-26
SULFURIC ACID	1.8E-28	3.0E-29	1.3E-33	8.7E-33	1.0E-30	7.8E-34	5.5E-23
SULFURIC ACID	8.5E-31	7.7E-32	1.7E-37	1.4E-36	7.5E-34	6.1E-38	1.1E-10
CYANOGENSULFIDE	4.1E-30	2.2E-28	3.1E-22	2.8E-34	5.6E-27	7.1E-22	0.
METHANETHIOL	1.0E-09	6.2E-09	5.4E-08	8.3E-10	3.4E-08	2.4E-07	0.
DIMETHYLSULFIDE	3.9E-15	1.3E-13	3.3E-11	2.4E-15	3.1E-12	2.4E-10	0.
DIMET.DISULFIDE	1.2E-20	5.1E-19	7.0E-16	5.9E-22	1.5E-17	8.1E-15	0.
ETHANETHIOL	5.9E-14	2.0E-12	4.9E-10	3.6E-14	4.7E-11	3.5E-09	0.
DIETHYLSULFIDE	1.2E-23	1.3E-20	2.4E-15	4.0E-24	5.1E-18	4.6E-14	0.
DIETH.DISULFIDE	5.3E-29	7.1E-26	7.4E-20	1.4E-30	3.6E-23	2.3E-18	0.
ETHANEDIITHIOL	1.1E-21	4.5E-20	6.1E-17	5.1E-23	1.3E-18	7.1E-16	0.
OCTANEETHIOL	0.	7.2E-36	8.3E-25	0.	9.0E-31	1.1E-22	0.
THIOFCRMIC ACID	1.5E-19	5.5E-19	4.4E-18	3.1E-22	8.5E-19	7.0E-18	0.
THIOACETIC ACID	5.5E-23	1.2E-21	2.6E-19	8.6E-26	7.4E-21	6.6E-19	0.
CYCLOPRCP.THICL	4.1E-19	8.9E-17	1.1E-11	1.3E-20	8.1E-15	7.4E-11	0.
CYCLOBUTA.THICL	2.4E-24	3.0E-21	9.9E-15	5.9E-26	1.1E-18	1.1E-13	0.
CYCLOCPT.THICL	1.2E-27	8.3E-24	7.7E-16	2.2E-29	1.3E-20	1.4E-14	0.
CYCLOHEXA.THICL	2.8E-29	1.1E-24	2.8E-15	3.9E-31	7.3E-21	8.5E-14	0.
M.SULFONIC ACID	2.9E-29	2.8E-29	3.4E-32	1.1E-33	3.9E-30	3.2E-32	0.
E.SULFINIC ACID	1.6E-13	3.0E-12	3.8E-11	3.5E-15	2.0E-11	1.6E-10	0.
THIOPHENNE	3.8E-21	5.9E-18	6.0E-09	4.7E-25	2.0E-15	2.5E-08	0.
BENZENETHIOL	9.0E-27	5.0E-22	6.9E-09	4.4E-32	2.7E-18	4.5E-08	0.
THIOCYANIC ACID	4.5E-17	3.5E-16	2.3E-13	3.9E-19	2.0E-15	5.8E-13	0.
THIOLGLYCOL	2.9E-25	5.3E-24	6.7E-23	6.2E-27	3.6E-23	2.9E-22	0.
CYSTEINE	9.6E-32	5.9E-30	4.7E-28	8.2E-36	5.5E-29	1.9E-27	0.
METHICNINE	0.	1.7E-38	1.1E-33	0.	2.8E-36	1.1E-32	0.

TABLE 25a

1000°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-50.753	-15.645	-4.291	-8.850	-57.421	-13.431	-43.183
2	2.0	9.0	89.0	-50.630	-14.851	-4.334	-8.831	-57.304	-14.187	-43.061
3	2.0	19.0	79.0	-50.424	-14.412	-4.409	-8.803	-57.102	-14.571	-42.855
4	2.0	29.0	69.0	-50.163	-14.121	-4.510	-8.774	-56.835	-14.804	-42.594
5	2.0	39.0	59.0	-49.811	-13.869	-4.656	-8.743	-56.455	-14.995	-42.241
6	2.0	49.0	49.0	-49.261	-13.601	-4.898	-8.710	-55.833	-15.196	-41.706
7	2.0	59.0	39.0	-47.940	-13.160	-5.523	-8.674	-54.252	-15.566	-40.370
8	2.0	69.0	29.0	-14.982	-4.954	-22.150	-8.702	-25.619	-23.837	-11.712
9	2.0	79.0	19.0	-12.785	-4.544	-23.560	-8.767	-23.537	-24.372	-12.662
10	2.0	89.0	9.0	-11.086	-4.361	-24.925	-8.825	-21.517	-24.668	-13.141
11	2.0	96.0	2.0	-0.625	-4.279	-35.245	-8.860	-9.049	-24.822	-13.378
12	10.0	2.0	88.0	-48.837	-15.547	-4.401	-8.806	-57.124	-13.442	-42.876
13	10.0	10.0	80.0	-48.640	-14.680	-4.477	-8.783	-56.924	-14.264	-42.679
14	10.0	20.0	70.0	-48.321	-14.238	-4.606	-8.753	-56.586	-14.644	-42.361
15	10.0	30.0	60.0	-47.850	-13.901	-4.809	-8.720	-56.062	-14.917	-41.890
16	10.0	40.0	50.0	-46.932	-13.511	-5.234	-8.685	-54.983	-15.238	-40.982
17	10.0	50.0	40.0	-14.583	-5.364	-21.470	-8.683	-26.629	-23.386	-10.856
18	10.0	60.0	30.0	-11.599	-4.730	-23.258	-8.750	-23.981	-24.151	-12.259
19	10.0	70.0	20.0	-9.958	-4.502	-24.507	-8.808	-22.136	-24.497	-12.832
20	10.0	80.0	10.0	-0.630	-4.371	-33.631	-8.860	-9.340	-24.729	-13.196
21	10.0	88.0	2.0	6.741	-4.295	-42.477	-8.964	-8.885	-24.671	-13.690
22	20.0	2.0	78.0	-47.550	-15.369	-4.638	-8.746	-56.501	-13.501	-42.282
23	20.0	10.0	70.0	-47.157	-14.451	-4.809	-8.720	-56.062	-14.367	-41.890
24	20.0	20.0	60.0	-46.238	-13.857	-5.234	-8.685	-54.983	-14.892	-40.971
25	20.0	30.0	50.0	-13.723	-5.583	-21.559	-8.683	-26.496	-23.166	-10.419
26	20.0	40.0	40.0	-10.783	-4.914	-23.337	-8.749	-23.862	-23.966	-11.889
27	20.0	50.0	30.0	-9.174	-4.663	-24.580	-8.808	-22.027	-24.335	-12.507
28	20.0	60.0	20.0	0.723	-4.515	-34.291	-8.860	-8.579	-24.589	-12.910
29	20.0	70.0	10.0	6.817	-4.408	-40.913	-8.939	-8.628	-24.531	-13.599
30	22.0	76.0	2.0	6.805	-4.310	-42.320	-9.849	-10.421	-26.057	-14.582
31	18.0	86.0	2.0	6.787	-4.305	-42.382	-8.887	-8.721	-24.518	-13.592
32	30.0	2.0	68.0	-45.474	-14.917	-5.406	-8.678	-54.548	-13.818	-40.622
33	30.0	10.0	60.0	-13.140	-6.094	-21.654	-8.683	-26.353	-22.656	-9.395
34	30.0	20.0	50.0	-10.256	-5.243	-23.417	-8.749	-23.743	-23.636	-11.308
35	30.0	30.0	40.0	-8.681	-4.912	-24.650	-8.808	-21.922	-24.087	-12.068
36	30.0	40.0	30.0	3.785	-4.717	-36.948	-8.867	-9.107	-24.385	-12.503
37	30.0	50.0	20.0	6.918	-4.592	-40.325	-8.929	-8.262	-24.349	-13.527
38	30.0	60.0	10.0	6.882	-4.452	-40.793	-8.837	-9.035	-24.300	-12.685
39	30.0	68.0	2.0	6.838	-4.327	-42.175	-8.743	-9.001	-24.241	-13.415
40	40.0	10.0	50.0	-8.311	-5.456	-24.717	-8.808	-21.822	-23.543	-11.134
41	40.0	20.0	40.0	1.216	-5.064	-34.090	-8.861	-8.984	-24.038	-11.981
42	40.0	30.0	30.0	7.081	-4.889	-46.085	-8.913	-8.944	-24.056	-13.489
43	40.0	40.0	20.0	7.025	-4.712	-40.246	-8.822	-8.898	-24.045	-13.419
44	40.0	50.0	10.0	6.952	-4.526	-40.635	-8.706	-8.842	-23.997	-12.308
45	40.0	58.0	2.0	6.883	-4.360	-41.939	-8.585	-8.787	-23.928	-13.226

TABLE 25b

1000°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	1.1E-13	3.0E-11	2.4E-10	6.7E-06	9.9E-03	8.8E-03	0.
H2	1.1E-01	2.7E-01	2.7E-01	8.0E-01	7.4E-01	6.8E-01	2.1E-09
O2	1.1E-15	2.7E-17	1.9E-18	3.1E-26	1.5E-32	1.8E-32	5.0E-01
WATER	6.0E-01	2.3E-01	6.2E-02	2.3E-05	1.5E-08	1.5E-08	2.5E-01
CO	3.3E-02	2.3E-01	5.1E-01	2.0E-01	2.4E-01	2.8E-01	1.6E-09
CO2	2.5E-01	2.7E-01	1.6E-01	7.9E-06	6.4E-09	8.7E-09	2.5E-01
BENZENE	0.	0.	0.	1.1E-23	2.3E-04	2.6E-04	0.
NAPHTHALENE	0.	0.	0.	8.9E-37	1.4E-04	2.0E-04	0.
ASPHALT	0.	0.	0.	0.	1.0E-02	2.5E-02	0.
ACETYLENE	3.1E-23	1.5E-19	1.0E-17	3.0E-10	8.2E-04	8.6E-04	0.
ETHYLENE	3.4E-25	4.2E-21	2.8E-19	2.4E-11	6.1E-05	5.9E-05	0.
ETHANE	2.2E-29	6.5E-25	4.4E-23	1.1E-14	2.6E-08	2.3E-08	0.
FORMIC ACID	4.0E-12	1.1E-11	6.3E-12	9.2E-16	6.9E-19	8.6E-19	7.8E-20
ACETIC ACID	4.3E-25	1.3E-22	6.1E-22	8.3E-22	1.0E-21	1.2E-21	0.
FORMALDEHYDE	9.5E-13	1.6E-11	3.6E-11	4.2E-11	4.6E-11	5.0E-11	8.7E-28
ACETALDEHYDE	3.4E-26	6.4E-23	1.2E-21	1.3E-17	2.2E-14	2.4E-14	0.
METHANOL	9.3E-19	3.9E-17	8.7E-17	3.0E-16	3.0E-16	3.1E-16	0.
ETHANOL	1.8E-33	8.2E-30	1.5E-28	4.8E-24	7.7E-21	7.6E-21	0.
N2	1.4E-04	1.3E-04	1.1E-04	1.0E-04	8.6E-05	1.1E-04	1.2E-04
NH3	4.7E-11	1.7E-10	1.6E-10	7.8E-10	6.5E-10	6.3E-10	1.2E-22
HCN	1.7E-14	1.1E-12	8.4E-12	4.3E-08	6.6E-05	7.5E-05	4.8E-33
NO	3.5E-14	5.0E-15	1.3E-15	1.5E-19	9.6E-23	1.2E-22	6.8E-07
NO2	1.8E-24	4.0E-26	2.8E-27	4.1E-35	0.	0.	7.5E-10
N2O	4.5E-22	6.2E-23	1.5E-23	1.7E-27	9.8E-31	1.4E-30	8.3E-15
NITROUS ACID	6.5E-24	2.3E-25	1.6E-26	4.0E-34	0.	0.	3.8E-13
NITRIC ACID	7.3E-35	4.0E-37	7.3E-39	0.	0.	0.	9.0E-17
C2N2	3.5E-31	6.2E-28	3.7E-26	3.2E-19	8.1E-13	1.1E-12	0.
HNCU	1.9E-14	1.9E-13	3.9E-13	2.5E-13	2.7E-13	3.4E-13	1.1E-25
P2	3.7E-20	9.4E-18	4.5E-16	3.9E-05	1.6E-04	7.1E-05	0.
P4O6	7.2E-05	6.3E-05	5.6E-05	1.6E-06	2.9E-24	1.2E-24	5.8E-13
P4O10	4.0E-26	2.0E-29	9.3E-32	0.	0.	0.	6.3E-05
PO	2.5E-12	6.2E-12	1.2E-11	4.3E-10	6.0E-13	4.5E-13	5.2E-18
PU2	3.1E-10	1.2E-10	6.0E-11	2.8E-13	2.7E-19	2.3E-19	1.4E-08
PH2	5.3E-13	2.1E-11	1.5E-10	1.3E-04	2.4E-04	1.5E-04	1.0E-33
PH3	1.8E-17	1.1E-15	7.8E-15	1.1E-08	2.1E-08	1.2E-08	0.
PCL3	2.1E-27	5.8E-27	2.8E-26	1.2E-21	4.4E-21	5.9E-21	5.0E-29
PUCL3	1.1E-26	4.7E-27	6.1E-27	3.2E-26	8.2E-29	1.2E-28	5.5E-21
PSCL3	5.3E-28	5.3E-28	2.1E-27	2.9E-23	7.3E-23	2.4E-22	0.
CL2	2.4E-17	7.6E-18	6.0E-18	1.7E-18	2.5E-18	3.9E-18	9.5E-10
HCL	2.9E-04	2.5E-04	2.3E-04	2.0E-04	2.4E-04	2.9E-04	2.5E-04
HOCL	2.0E-16	2.7E-17	6.4E-18	7.2E-22	5.9E-25	8.0E-25	3.6E-09
CL2O	9.8E-34	4.8E-35	1.0E-35	0.	0.	0.	8.1E-19
CH3CL	9.7E-21	9.4E-19	6.8E-18	5.7E-14	1.1E-10	1.3E-10	0.
CH2CL2	1.8E-28	6.3E-27	4.1E-26	1.0F-22	2.5E-19	3.9E-19	0.
CHCL3	1.6E-36	2.0E-35	1.1E-34	8.8E-32	2.6E-28	5.4E-28	0.
CCL4	0.	0.	0.	0.	3.4E-38	9.3E-38	0.
COCL2	6.1E-24	1.3E-23	2.3E-23	2.5E-24	4.4E-24	8.4E-24	1.1E-23
S2	1.9E-06	2.4E-07	1.6E-07	1.7E-08	7.7E-09	4.8E-08	8.0E-34
S8	2.1E-37	0.	0.	0.	0.	0.	0.
H2S	2.9E-04	2.5E-04	2.1E-04	2.0E-04	1.3E-04	2.9E-04	1.2E-25
SU2	2.7E-05	2.3E-07	1.4E-08	7.2E-17	2.3E-23	7.2E-23	2.5E-04
S03	2.5E-14	3.3E-17	5.4E-19	3.5E-31	0.	0.	4.9E-06
CUS	2.8E-06	6.9E-06	1.3E-05	1.6E-06	1.3E-06	3.8E-06	2.7E-27
CS2	7.0E-12	4.0E-11	2.3E-10	7.5E-08	5.7E-05	3.8E-04	0.
SU	1.5E-07	8.4E-09	1.9E-09	7.7E-14	3.5E-17	1.0E-16	6.7E-14
SULFURCUS ACID	1.3E-22	4.2E-25	6.9E-27	1.3E-38	0.	0.	5.0E-22
SULFURIC ACID	1.1E-24	5.5E-28	2.4E-30	0.	0.	0.	8.8E-17
CYANOGENSULFIDE	5.4E-35	3.4E-32	1.7E-30	4.9E-24	8.1E-18	2.8E-17	0.
METHANEETHYL	4.6E-20	4.4E-18	3.0E-17	2.7E-13	2.6E-10	5.9E-10	0.
DIMETHYLSULFIDE	4.6E-36	4.9E-32	2.8E-30	2.3E-22	3.6E-16	7.8E-16	0.
DIMET.CISULFIDE	0.	1.1E-37	5.1E-36	1.3E-28	1.4E-22	7.7E-22	0.
ETHANETHIOL	4.5E-35	4.8E-31	2.7E-29	2.2E-21	3.5E-15	7.6E-15	0.
DIETHYLSULFIDE	0.	0.	0.	1.4E-38	5.4E-26	1.1E-25	0.
DIETH.CISULFIDE	0.	0.	0.	0.	2.6E-32	1.4E-31	0.
ETHANECITHIOL	0.	4.2E-38	2.0E-36	5.3E-29	5.6E-23	3.0E-22	0.
OCTANETHIOL	0.	0.	0.	0.	0.	0.	0.
THIOFORMIC ACID	8.4E-21	5.1E-20	9.4E-20	3.6E-20	2.6E-20	7.2E-20	0.
THIODACETIC ACID	3.0E-37	2.0E-34	3.0E-33	1.1E-29	1.2E-26	3.3E-26	0.
CYCLOPROP.THIOL	0.	1.9E-37	8.7E-35	2.2E-23	6.0E-14	1.4E-13	0.
CYCLOBUTA.THIOL	0.	0.	0.	2.0E-32	8.7E-20	2.0E-19	0.
CYCLOPENT.THIOL	0.	0.	0.	0.	8.1E-26	1.8E-25	0.
CYCLOHEXA.THIOL	0.	0.	0.	0.	1.2E-27	2.5E-27	0.
M.SULFCNIC ACID	1.4E-35	5.1E-36	6.8E-37	0.	0.	0.	0.
E.SULFINIC ACID	7.8E-37	1.3E-33	2.0E-32	2.0E-28	2.2E-25	5.4E-25	0.
THIOPHEN	0.	6.5E-39	2.4E-35	6.7E-21	3.3E-08	9.0E-08	0.
BENZENETHIOL	0.	0.	0.	1.0E-29	1.4E-10	3.9E-10	0.
THIOCYANIC ACID	2.5E-19	5.8E-18	3.8E-17	6.2E-14	6.4E-11	1.8E-10	0.
THIOLGLYCC	0.	0.	0.	2.2E-35	2.4E-32	5.9E-32	0.
CYSTEINE	0.	0.	0.	0.	0.	0.	0.
METHIONINE	0.	0.	0.	0.	0.	0.	0.

TABLE 26a

1000°K AND 0.2 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-50.753	-13.918	-0.837	-5.396	-64.329	-8.254	-43.791
2	2.0	9.0	89.0	-50.630	-13.124	-0.880	-5.377	-64.212	-9.011	-43.649
3	2.0	19.0	79.0	-50.424	-12.685	-0.956	-5.350	-64.009	-9.395	-43.410
4	2.0	29.0	69.0	-50.163	-12.394	-1.057	-5.320	-63.742	-9.625	-43.108
5	2.0	39.0	59.0	-49.811	-12.142	-1.202	-5.289	-63.363	-9.816	-42.699
6	2.0	49.0	49.0	-49.261	-11.874	-1.444	-5.256	-62.741	-10.018	-42.067
7	2.0	59.0	39.0	-47.939	-11.433	-2.070	-5.220	-61.160	-10.389	-40.588
8	2.0	69.0	29.0	-8.074	-1.500	-22.150	-5.249	-23.892	-20.379	-11.719
9	2.0	79.0	19.0	-5.878	-1.090	-23.560	-5.314	-21.809	-20.917	-12.666
10	2.0	89.0	9.0	-4.186	-0.907	-24.923	-5.371	-19.793	-21.216	-13.144
11	2.0	96.0	2.0	-0.964	-0.829	-28.168	-5.402	-14.941	-21.354	-13.361
12	10.0	2.0	88.0	-48.837	-13.820	-0.947	-5.352	-64.032	-8.266	-43.436
13	10.0	10.0	80.0	-48.640	-12.953	-1.023	-5.329	-63.831	-9.085	-43.207
14	10.0	20.0	70.0	-48.321	-12.511	-1.152	-5.299	-63.493	-9.466	-42.837
15	10.0	30.0	60.0	-47.850	-12.174	-1.355	-5.266	-62.970	-9.738	-42.294
16	10.0	40.0	50.0	-46.931	-11.784	-1.780	-5.231	-61.890	-10.060	-41.253
17	10.0	50.0	40.0	-7.675	-1.911	-21.470	-5.229	-24.901	-19.927	-10.859
18	10.0	60.0	30.0	-4.691	-1.276	-23.258	-5.296	-22.255	-20.696	-12.261
19	10.0	70.0	20.0	-3.051	-1.048	-24.507	-5.356	-20.410	-21.043	-12.835
20	10.0	80.0	10.0	0.124	-0.926	-27.536	-5.393	-15.885	-21.240	-13.154
21	10.0	88.0	2.0	2.989	-0.958	-31.686	-5.273	-9.599	-20.958	-12.841
22	20.0	2.0	78.0	-47.550	-13.642	-1.185	-5.292	-63.408	-8.323	-42.747
23	20.0	10.0	70.0	-47.157	-12.724	-1.355	-5.266	-62.970	-9.188	-42.294
24	20.0	20.0	60.0	-46.238	-12.130	-1.780	-5.231	-61.890	-9.713	-41.253
25	20.0	30.0	50.0	-6.815	-2.129	-21.559	-5.229	-24.768	-19.711	-10.453
26	20.0	40.0	40.0	-3.875	-1.460	-23.337	-5.296	-22.135	-20.513	-11.917
27	20.0	50.0	30.0	-2.266	-1.209	-24.580	-5.354	-20.301	-20.882	-12.533
28	20.0	60.0	20.0	0.821	-1.077	-27.507	-5.393	-15.929	-21.086	-12.849
29	20.0	70.0	10.0	4.376	-1.229	-31.374	-5.237	-10.047	-20.609	-12.238
30	22.0	76.0	2.0	5.435	-1.331	-33.693	-5.914	-8.955	-21.778	-13.295
31	18.0	80.0	2.0	5.288	-1.296	-33.638	-5.117	-6.583	-20.278	-11.822
32	30.0	2.0	68.0	-45.474	-13.190	-1.952	-5.224	-61.456	-8.639	-40.855
33	30.0	10.0	60.0	-6.232	-2.640	-21.654	-5.228	-24.626	-19.198	-9.396
34	30.0	20.0	50.0	-3.348	-1.789	-23.417	-5.295	-22.016	-20.180	-11.233
35	30.0	30.0	40.0	-1.774	-1.458	-24.650	-5.354	-20.196	-20.631	-12.013
36	30.0	40.0	30.0	1.490	-1.288	-27.754	-5.395	-15.559	-20.879	-12.482
37	30.0	50.0	20.0	5.475	-1.564	-31.816	-5.268	-9.392	-29.308	-11.662
38	30.0	60.0	10.0	5.538	-1.469	-32.303	-5.134	-8.595	-20.133	-11.506
39	30.0	68.0	2.0	5.518	-1.363	-33.608	-4.991	-7.187	-19.957	-11.443
40	40.0	10.0	50.0	-1.403	-2.002	-24.717	-5.354	-20.095	-20.088	-11.137
41	40.0	20.0	40.0	2.394	-1.644	-28.363	-5.400	-14.649	-20.534	-11.857
42	40.0	30.0	30.0	5.693	-1.820	-31.713	-5.311	-9.568	-20.138	-11.328
43	40.0	40.0	20.0	5.678	-1.693	-31.870	-5.194	-9.297	-20.032	-11.194
44	40.0	50.0	10.0	5.635	-1.548	-32.210	-5.037	-8.686	-19.866	-11.218
45	40.0	58.0	2.0	5.585	-1.406	-33.420	-4.861	-7.096	-19.659	-11.092

TABLE 26b

1000°K AND 0.2 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	1.1E-07	3.0E-05	2.4E-04	1.4E-02	2.9E-01	3.5E-01	0.
H2	1.1E-01	2.7E-01	2.7E-01	7.8E-01	4.3E-01	2.6E-01	6.8E-11
O2	1.1E-18	2.7E-20	1.9E-21	6.0E-24	2.8E-27	4.4E-28	5.0E-01
WATER	6.0E-01	2.3E-01	6.2E-02	1.0E-02	1.2E-04	2.9E-05	2.5E-01
CO	3.3E-02	2.3E-01	5.1E-01	1.9E-01	2.9E-01	3.6E-01	4.9E-11
CO2	2.5E-01	2.7E-01	1.6E-01	3.3E-03	1.1E-04	5.4E-05	2.5E-01
BENZENE	1.3E-38	1.5E-27	4.6E-22	9.8E-16	1.9E-05	4.9E-03	0.
NAPHTHALENE	0.	0.	1.3E-34	1.5E-24	4.0E-07	6.5E-03	0.
ASPHALT	0.	0.	0.	0.	1.8E-12	1.3E-02	0.
ACETYLENE	3.1E-17	1.5E-13	1.0E-11	1.3E-09	3.6E-06	2.3E-05	0.
ETHYLENE	3.4E-16	4.2E-12	2.8E-10	1.0E-07	1.5E-04	6.0E-04	0.
ETHANE	2.2E-17	6.5E-13	4.4E-11	4.8E-08	3.8E-05	9.3E-05	0.
FORMIC ACID	4.0E-09	1.1E-08	6.3E-09	3.8E-10	6.7E-12	2.1E-12	2.5E-18
ACETIC ACID	4.3E-16	1.3E-13	6.1E-13	7.1E-13	4.8E-13	3.0E-13	0.
FORMALDEHYDE	9.5E-10	1.6E-08	3.6E-08	3.8E-08	3.2E-08	2.5E-08	8.8E-28
ACETALDEHYDE	3.4E-17	6.4E-14	1.2E-12	2.4E-11	7.7E-10	1.2E-09	0.
METHANOL	9.3E-13	3.9E-11	8.7E-11	2.7E-10	1.2E-10	5.9E-11	0.
ETHANOL	1.8E-21	8.2E-18	1.5E-16	9.0E-15	1.6E-13	1.5E-13	0.
N2	1.4E-04	1.3E-04	1.1E-04	1.0E-04	1.4E-04	1.7E-04	1.2E-04
NH3	4.7E-08	1.7E-07	1.6E-07	7.7E-07	3.6E-07	2.0E-07	6.8E-22
HCN	1.7E-11	1.1E-09	8.4E-09	9.2E-08	5.6E-06	1.6E-05	8.6E-34
NO	1.1E-15	1.6E-16	4.0E-17	2.1E-18	5.4E-20	2.4E-20	6.8E-07
NO2	5.7E-26	1.3E-27	8.7E-29	2.6E-31	1.4E-34	2.5E-35	2.4E-08
N2O	4.5E-22	6.2E-23	1.5E-23	7.6E-25	2.2E-26	1.1E-26	2.6E-13
NITROUS ACID	6.5E-24	2.3E-25	1.6E-26	8.0E-29	3.3E-32	4.3E-33	6.7E-11
NITRIC ACID	7.3E-35	4.0E-37	7.3E-39	0.	0.	0.	5.0E-13
C2N2	3.5E-25	6.2E-22	3.7E-20	1.5E-18	1.0E-14	1.3E-13	0.
HNC	1.9E-11	1.9E-10	3.9E-10	2.4E-10	3.1E-10	3.5E-10	6.5E-25
P2	1.2E-21	3.0E-19	1.4E-17	8.0E-14	9.4E-09	1.7E-07	0.
P4O6	7.2E-05	6.3E-05	5.6E-05	5.2E-05	7.2E-05	9.1E-05	5.8E-19
P4O10	4.0E-26	2.0E-29	9.3E-32	8.3E-37	0.	0.	6.3E-05
PO	1.4E-14	3.5E-14	6.5E-14	2.7E-13	2.0E-12	3.4E-12	1.6E-22
PO2	1.8E-12	6.7E-13	3.4E-13	7.8E-14	1.2E-14	8.3E-15	1.4E-11
PH2	3.0E-12	1.2E-10	8.2E-10	1.8E-07	3.3E-05	8.8E-05	3.2E-38
PH3	3.2E-15	2.0E-13	1.4E-12	5.1E-10	7.0E-08	1.5E-07	0.
PCL3	3.8E-25	1.0E-24	5.0E-24	6.0E-23	1.4E-19	2.4E-18	2.8E-28
POCL3	1.9E-24	8.3E-25	1.1E-24	7.3E-25	3.6E-23	2.5E-22	9.6E-19
PSCL3	9.6E-26	9.1E-26	4.0E-25	1.6E-24	8.8E-21	3.3E-19	0.
CL2	2.5E-17	7.6E-18	6.0E-18	1.8E-18	6.3E-18	1.6E-17	3.0E-08
HCl	2.9E-04	2.5E-04	2.3E-04	2.1E-04	2.9E-04	3.7E-04	2.5E-04
HOC	2.0E-16	2.7E-17	6.4E-18	3.3E-19	9.9E-21	4.9E-21	1.1E-07
CL2O	9.9E-34	4.8E-35	1.0E-35	1.7E-37	1.3E-38	1.3E-38	8.1E-16
CH3CL	9.7E-15	9.4E-13	6.8E-12	1.2E-10	6.5E-09	1.6E-08	0.
CH2CL2	1.9E-22	6.3E-21	4.1E-20	2.3E-19	3.2E-17	1.6E-16	0.
CHCL3	1.6E-30	2.0E-29	1.1E-28	2.0E-28	7.1E-26	7.4E-25	3.8E-39
CCL4	0.	7.5E-39	3.8E-38	2.2E-38	2.0E-35	4.2E-34	5.8E-39
COCL2	6.2E-21	1.3E-20	2.3E-20	2.5E-21	1.4E-20	4.4E-20	1.1E-20
S2	1.8E-09	2.2E-10	1.8E-10	1.9E-11	1.2E-10	5.1E-10	3.1E-37
S8	0.	0.	0.	0.	0.	0.	0.
H2S	2.9E-04	2.5E-04	2.3E-04	2.1E-04	2.8E-04	3.7E-04	2.3E-27
SO2	2.7E-08	2.3E-10	1.5E-11	1.5E-14	1.7E-17	5.6E-18	1.6E-04
SU3	2.5E-17	3.2E-20	5.7E-22	3.1E-26	7.9E-31	1.0E-31	9.6E-05
CUS	2.8E-06	6.7E-06	1.3E-05	1.6E-06	6.0E-06	1.6E-05	5.4E-29
CS2	7.0E-12	3.8E-11	2.5E-10	1.7E-10	7.6E-08	1.0E-06	0.
SO	1.5E-10	8.2E-12	2.0E-12	3.6E-14	1.9E-15	1.6E-15	1.3E-15
SULFURIC ACID	1.3E-22	4.1E-25	7.3E-27	1.2E-30	1.6E-35	1.3E-36	3.1E-19
SULFURIC ACID	1.1E-24	5.3E-28	2.6E-30	3.3E-35	0.	0.	1.7E-12
CYANOGENSULFIDE	5.4E-29	3.3E-26	1.8E-24	2.3E-23	4.0E-19	1.0E-17	0.
METHANETHIOL	4.5E-14	4.3E-12	3.2E-11	5.7E-10	3.0E-08	7.6E-08	0.
DIMETHYLSULFIDE	4.6E-24	4.8E-20	2.9E-18	1.0E-15	2.0E-12	1.0E-11	0.
DIMET.CISULFIDE	2.8E-29	1.0E-25	5.7E-24	6.2E-22	3.1E-18	3.3E-17	0.
ETHANETHIOL	4.5E-23	4.6E-19	2.8E-17	9.8E-15	2.0E-11	9.9E-11	0.
DIETHYLSULFIDE	0.	4.9E-34	2.0E-30	2.6E-25	7.7E-19	1.5E-17	0.
DIETH.CISULFIDE	0.	0.	4.8E-36	2.0E-31	1.4E-24	5.9E-23	0.
ETHANECHITHIOL	1.1E-29	4.0E-26	2.2E-24	2.5E-22	1.2E-18	1.3E-17	0.
OCTANETHIOL	0.	0.	0.	0.	2.4E-32	7.1E-30	0.
THIOFORMIC ACID	8.4E-18	5.0E-17	1.0E-16	3.4E-17	7.1E-17	1.2E-16	0.
THIOACETIC ACID	3.0E-28	1.9E-25	3.2E-24	2.1E-23	1.7E-21	5.4E-21	0.
CYCLOPROP.THIOL	3.9E-28	1.8E-22	9.2E-20	2.1E-16	3.0E-11	4.8E-10	0.
CYCLOBUTA.THIOL	4.3E-38	2.2E-30	9.0E-27	4.0E-22	2.2E-15	6.9E-14	0.
CYCLOPENT.ThiOL	0.	1.7E-38	5.7E-34	4.9E-28	1.0E-19	6.3E-18	0.
CYCLOHEXA.THIOL	0.	0.	5.5E-37	9.1E-30	7.3E-20	9.0E-18	0.
M.SULFONIC ACID	1.4E-29	4.9E-30	7.2E-31	2.2E-33	1.2E-36	1.8E-37	0.
E.SULFINIC ACID	7.8E-25	1.2E-21	2.1E-20	4.0E-19	1.7E-17	3.4E-17	0.
THIOPHENE	7.5E-31	6.3E-24	2.6E-20	1.4E-16	2.5E-09	2.1E-07	0.
BENZENETHIOL	0.	4.4E-33	1.3E-27	9.0E-22	4.4E-11	2.3E-08	0.
THIOCYANIC ACID	2.5E-16	5.7E-15	4.0E-14	1.4E-13	2.1E-11	1.2E-10	0.
THIOLGLYCOL	8.6E-32	1.4E-28	2.3E-27	4.4E-26	1.9E-24	3.8E-24	0.
CYSTEINE	0.	0.	3.7E-38	4.3E-37	2.4E-35	5.3E-35	0.
METHIONINE	0.	0.	0.	0.	0.	0.	0.

TABLE 27a

1000°K AND 20 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{\partial F}{\partial n_i}$ /RT, FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-50.753	-12.767	1.466	-3.094	-68.934	-4.803	-45.300
2	2.0	9.0	89.0	-50.630	-11.973	1.423	-3.075	-68.817	-5.553	-45.252
3	2.0	19.0	79.0	-50.424	-11.534	1.347	-3.047	-68.614	-5.938	-44.980
4	2.0	29.0	69.0	-50.163	-11.243	1.246	-3.018	-68.347	-6.171	-44.631
5	2.0	39.0	59.0	-49.810	-10.991	1.100	-2.987	-67.968	-6.361	-44.152
6	2.0	49.0	49.0	-49.260	-10.723	0.858	-2.953	-67.346	-6.564	-43.399
7	2.0	59.0	39.0	-47.938	-10.282	0.232	-2.918	-65.764	-6.935	-41.597
8	2.0	69.0	29.0	-3.614	0.783	-22.097	-2.970	-22.818	-18.048	-11.675
9	2.0	79.0	19.0	-2.681	1.142	-23.248	-3.063	-21.111	-18.484	-12.468
10	2.0	89.0	9.0	-3.191	1.350	-24.454	-3.186	-19.325	-18.784	-12.976
11	2.0	96.0	2.0	-3.633	1.452	-26.234	-3.289	-16.673	-18.965	-13.255
12	10.0	2.0	88.0	-48.837	-12.669	1.356	-3.050	-68.637	-4.814	-45.009
13	10.0	10.0	80.0	-48.640	-11.801	1.280	-3.027	-68.436	-5.630	-44.745
14	10.0	20.0	70.0	-48.321	-11.360	1.151	-2.996	-68.098	-6.011	-44.315
15	10.0	30.0	60.0	-47.850	-11.023	0.948	-2.964	-67.574	-6.284	-43.672
16	10.0	40.0	50.0	-46.931	-10.632	0.522	-2.929	-66.494	-6.606	-42.413
17	10.0	50.0	40.0	-3.127	0.379	-21.441	-2.934	-23.793	-17.611	-10.833
18	10.0	60.0	30.0	-1.094	0.857	-22.703	-2.979	-21.910	-18.131	-11.828
19	10.0	70.0	20.0	-0.649	1.001	-23.250	-2.979	-21.080	-18.235	-12.087
20	10.0	80.0	10.0	-0.614	1.130	-23.944	-2.979	-20.029	-18.321	-12.294
21	10.0	88.0	2.0	-1.072	1.286	-25.682	-3.034	-17.428	-18.500	-12.627
22	20.0	2.0	78.0	-47.550	-12.490	1.118	-2.990	-68.013	-4.873	-44.208
23	20.0	10.0	70.0	-47.157	-11.573	0.948	-2.964	-67.574	-5.734	-43.672
24	20.0	20.0	60.0	-46.238	-10.979	0.522	-2.929	-66.494	-6.260	-42.412
25	20.0	30.0	50.0	-2.263	0.161	-21.531	-2.930	-23.659	-17.393	-10.395
26	20.0	40.0	40.0	-0.178	0.637	-22.772	-2.960	-21.805	-17.900	-11.383
27	20.0	50.0	30.0	0.463	0.740	-23.266	-2.943	-21.054	-17.961	-11.569
28	20.0	60.0	20.0	0.955	0.777	-23.741	-2.903	-20.320	-17.915	-11.598
29	20.0	70.0	10.0	1.573	0.753	-24.487	-2.836	-19.170	-17.764	-11.381
30	22.0	76.0	2.0	4.734	0.100	-28.266	-3.505	-13.840	-18.456	-11.448
31	18.0	80.0	2.0	1.662	0.813	-25.779	-2.777	-17.200	-17.698	-11.355
32	30.0	2.0	68.0	-45.473	-12.039	0.350	-2.921	-66.060	-5.185	-41.924
33	30.0	10.0	60.0	-1.640	-0.341	-21.647	-2.926	-23.485	-16.890	-9.526
34	30.0	20.0	50.0	0.727	0.309	-23.062	-2.959	-21.378	-17.604	-10.857
35	30.0	30.0	40.0	1.573	0.397	-23.670	-2.955	-20.460	-17.669	-11.014
36	30.0	40.0	30.0	2.421	0.349	-24.353	-2.926	-19.423	-17.566	-10.892
37	30.0	50.0	20.0	4.154	0.037	-25.925	-2.883	-17.044	-17.172	-10.324
38	30.0	60.0	10.0	4.943	-0.064	-27.041	-2.755	-15.306	-16.811	-9.835
39	30.0	68.0	2.0	4.948	0.029	-28.318	-2.603	-13.314	-16.599	-9.537
40	40.0	10.0	50.0	2.823	-0.196	-24.390	-3.016	-19.415	-17.210	-10.335
41	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
42	40.0	30.0	30.0	5.102	-0.388	-26.519	-2.946	-16.184	-16.873	-10.040
43	40.0	40.0	20.0	5.107	-0.283	-26.678	-2.826	-15.886	-16.737	-9.842
44	40.0	50.0	10.0	5.076	-0.155	-26.999	-2.665	-15.325	-16.544	-9.564
45	40.0	58.0	2.0	5.035	-0.025	-28.144	-2.480	-13.514	-16.301	-9.211

TABLE 27b

1000°K AND 20 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.01% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	9.8E-04	5.3E-02	1.2E-01	2.4E-01	4.8E-01	5.3E-01	0.
H2	1.1E-01	1.8E-01	1.1E-01	4.8E-01	2.3E-01	4.4E-02	6.8E-12
O2	1.2E-20	8.3E-22	1.4E-22	8.0E-23	2.7E-23	1.6E-25	5.0E-01
WATER	6.1E-01	2.7E-01	6.8E-02	2.2E-01	6.1E-02	9.2E-04	2.5E-01
CO	3.2E-02	1.6E-01	3.8E-01	3.3E-02	1.7E-01	3.8E-01	4.9E-12
CO2	2.5E-01	3.4E-01	3.2E-01	2.1E-02	6.3E-02	1.1E-02	2.5E-01
BENZENE	8.4E-23	1.9E-14	1.7E-10	2.7E-14	1.4E-09	6.3E-03	0.
NAPHTHALENE	4.1E-36	2.0E-22	1.2E-15	1.3E-22	2.1E-14	1.3E-02	0.
ASPHALT	0.	0.	8.8E-33	0.	6.3E-31	5.5E-03	0.
ACETYLENE	2.7E-13	1.7E-10	3.4E-09	1.9E-10	7.0E-09	1.1E-06	0.
ETHYLENE	2.9E-10	3.0E-07	3.8E-06	9.0E-07	1.6E-05	5.1E-04	0.
ETHANE	1.8E-09	3.1E-06	2.4E-05	2.5E-05	2.1E-04	1.3E-03	0.
FORMIC ACID	3.9E-07	8.7E-07	5.2E-07	1.5E-07	2.1E-07	7.1E-09	2.5E-17
ACETIC ACID	3.9E-10	2.8E-08	5.8E-08	8.0E-09	4.7E-08	9.2E-09	0.
FORMALDEHYDE	9.0E-08	7.6E-07	1.1E-06	4.1E-07	9.9E-07	4.4E-07	8.8E-28
ACETALDEHYDE	3.0E-11	8.1E-09	4.2E-08	7.5E-09	7.6E-08	1.9E-07	0.
METHANOL	8.6E-09	1.2E-07	1.1E-07	1.7E-07	2.0E-07	1.7E-08	5.3E-39
ETHANOL	1.5E-13	6.9E-11	2.2E-10	1.7E-10	8.2E-10	4.0E-10	0.
N2	1.4E-04	1.3E-04	1.4E-04	1.3E-04	1.7E-04	2.0E-04	1.2E-04
NH3	4.5E-06	9.5E-06	4.7E-06	4.1E-05	1.5E-05	1.4E-06	2.2E-21
HCN	1.5E-09	3.7E-08	1.7E-07	3.8E-08	2.7E-07	3.8E-06	2.7E-34
NO	1.1E-16	2.9E-17	1.2E-17	8.7E-18	5.9E-18	4.9E-19	6.8E-07
NO2	6.0E-27	4.1E-28	6.8E-29	3.9E-29	1.5E-29	9.8E-32	2.4E-07
N2O	4.6E-22	1.2E-22	4.8E-23	3.5E-23	2.7E-23	2.4E-24	2.6E-12
NITROUS ACID	6.8E-24	5.9E-25	7.8E-26	9.2E-26	2.5E-26	7.1E-29	2.1E-09
NITRIC ACID	7.8E-35	1.8E-36	9.7E-38	8.7E-38	1.4E-38	0.	1.6E-10
C2N2	3.1E-21	1.1E-18	3.6E-17	4.3E-19	4.5E-17	4.5E-14	0.
HNCO	1.8E-09	1.1E-08	2.1E-08	3.6E-09	1.5E-08	1.6E-08	2.0E-24
P2	1.1E-22	5.7E-21	8.5E-20	2.0E-19	1.1E-18	2.5E-15	0.
P4O6	7.3E-05	7.0E-05	6.9E-05	7.5E-05	9.0E-05	1.0E-04	5.8E-23
P4O10	4.5E-26	2.1E-28	5.8E-30	2.1E-30	2.9E-31	1.2E-35	6.3E-05
PU	4.4E-16	8.5E-16	1.3E-15	1.6E-15	2.1E-15	8.0E-15	1.6E-25
PO2	5.7E-14	2.9E-14	1.8E-14	1.6E-14	1.3E-14	3.8E-15	1.4E-13
PH2	8.9E-12	1.1E-10	2.6E-10	1.7E-09	1.9E-09	1.8E-08	0.
PH3	9.4E-14	1.5E-12	2.8E-12	3.8E-11	2.9E-11	1.2E-10	0.
PCl3	1.2E-23	3.6E-23	2.8E-22	6.1E-23	7.6E-22	6.3E-19	8.8E-28
POCl3	6.3E-23	5.1E-23	1.6E-22	2.7E-23	1.9E-22	1.3E-20	3.1E-17
PSCl3	3.1E-24	5.5E-24	6.1E-23	3.7E-24	1.2E-22	4.5E-19	0.
Cl2	2.5E-17	1.4E-17	2.2E-17	6.1E-18	1.9E-17	1.3E-16	3.0E-07
HCl	2.9E-04	2.8E-04	2.8E-04	3.0E-04	3.6E-04	4.1E-04	2.5E-04
HOCl	2.0E-16	5.2E-17	2.1E-17	1.7E-17	1.2E-17	1.1E-18	1.1E-06
Cl2O	1.1E-33	1.6E-34	1.0E-34	2.1E-35	3.7E-35	1.9E-35	8.1E-14
CH3CL	9.0E-11	2.8E-09	9.8E-09	5.2E-09	2.6E-08	1.7E-07	0.
CH2CL2	1.8E-18	3.1E-17	1.8E-16	2.4E-17	3.0E-16	1.1E-14	3.1E-38
CHCl3	1.6E-26	1.6E-25	1.5E-24	4.9E-26	1.6E-24	3.5E-22	3.8E-36
CCl4	1.7E-35	1.0E-34	1.5E-33	1.3E-35	1.0E-33	1.4E-30	5.8E-35
COCl2	6.2E-19	1.8E-18	6.5E-18	1.5E-19	2.4E-18	3.6E-17	1.1E-18
S2	1.9E-11	6.5E-12	1.4E-11	1.0E-12	6.5E-12	1.4E-10	0.
S8	0.	0.	0.	0.	0.	7.5E-39	0.
H2S	2.9E-04	2.8E-04	2.5E-04	3.0E-04	3.5E-04	3.2E-04	5.3E-29
SO2	3.0E-10	1.2E-11	2.9E-12	4.6E-13	3.9E-13	1.1E-14	3.6E-05
SO3	2.8E-19	3.0E-21	2.9E-22	3.6E-23	1.7E-23	3.8E-26	2.2E-04
COS	2.8E-06	8.1E-06	2.7E-05	6.5E-07	8.4E-06	8.9E-05	1.2E-30
CS2	6.9E-12	4.4E-11	5.3E-10	4.6E-12	2.5E-10	1.6E-07	0.
SO	1.6E-12	2.5E-13	1.4E-13	3.1E-14	4.4E-14	1.6E-14	3.0E-17
SULFURIC ACID	1.4E-22	2.5E-24	1.5E-25	8.1E-26	1.9E-26	8.0E-30	7.1E-18
SULFURIC ACID	1.2E-24	5.8E-27	1.4E-28	5.7E-29	7.7E-30	2.6E-34	4.0E-10
CYANOGENSULFIDE	4.9E-25	9.8E-23	4.7E-21	1.6E-23	4.2E-21	1.9E-17	0.
METHANETHIOL	4.2E-10	1.3E-08	4.1E-08	2.4E-08	1.2E-07	6.2E-07	0.
DIMETHYLSULFIDE	3.9E-16	3.9E-13	4.4E-12	1.2E-12	2.6E-11	7.6E-10	0.
DIMET.CISULFIDE	2.5E-21	1.4E-18	2.3E-17	1.8E-18	9.3E-17	1.3E-14	0.
ETHANETHIOL	3.8E-15	3.7E-12	4.3E-11	1.2E-11	2.5E-10	7.4E-09	0.
DIETHYLSULFIDE	2.8E-26	2.8E-20	4.1E-18	2.8E-19	1.0E-16	9.5E-14	0.
DIETH.CISULFIDE	2.2E-31	1.3E-25	2.6E-23	4.9E-25	4.4E-22	2.0E-18	0.
ETHANECITHIOL	9.7E-22	5.5E-19	9.1E-18	7.2E-19	3.7E-17	5.1E-15	0.
OCTANEIHC10L	0.	3.2E-35	7.6E-31	2.8E-33	3.1E-28	3.1E-22	0.
THIOFORMIC ACID	8.2E-16	4.0E-15	8.4E-15	8.6E-16	5.2E-15	1.1E-14	0.
THIOACETIC ACID	2.7E-22	4.1E-20	3.1E-19	1.6E-20	3.9E-19	4.6E-18	0.
CYCLOCPRCP.IIIOL	3.2E-18	6.0E-14	3.9E-12	1.2E-13	2.3E-11	2.0E-08	0.
CYCLOBUTA.THOL	3.2E-24	1.9E-18	4.4E-16	6.9E-18	5.3E-15	2.6E-11	0.
CYCLOPENT.THIOL	2.0E-30	3.9E-23	3.3E-20	2.4E-22	7.9E-19	2.2E-14	0.
CYCLOHEXA.THOL	2.0E-32	1.2E-23	3.7E-20	1.3E-22	1.8E-18	2.9E-13	0.
M.SULFCVIC ACID	1.4E-25	8.1E-26	1.7E-26	4.5E-27	4.3E-27	1.1E-29	0.
E.SULFINIC ACID	6.8E-17	1.8E-14	8.2E-14	1.8E-14	2.1E-13	4.9E-13	0.
THIOPHENE	5.8E-21	1.2E-15	7.6E-13	6.3E-16	2.2E-12	2.8E-07	0.
BENZENEIHC10L	7.9E-28	1.0E-19	1.3E-15	5.8E-20	7.6E-15	1.6E-07	0.
THIOCYANIC ACID	2.4E-14	3.3E-13	2.2E-12	1.4E-13	2.4E-12	1.6E-10	0.
THIOLGLYCOL	7.5E-24	2.0E-21	9.1E-21	2.0E-21	2.3E-20	5.4E-20	0.
CYSTEINE	5.5E-32	9.1E-29	7.8E-28	2.9E-29	1.4E-27	3.6E-27	0.
METHIONINE	0.	3.9E-37	4.3E-35	3.8E-37	3.3E-34	2.6E-32	0.

TABLE 28a

300°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\bar{F}_i/RT$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-161.300	-49.874	-4.291	-11.150	-281.849	-11.278	-173.240
2	2.0	9.0	89.0	-161.178	-49.082	-4.333	-11.132	-281.733	-11.408	-173.074
3	2.0	19.0	79.0	-160.971	-48.643	-4.409	-11.104	-281.530	-11.516	-172.792
4	2.0	29.0	69.0	-160.711	-48.352	-4.510	-11.075	-281.263	-11.602	-172.431
5	2.0	39.0	52.0	-160.359	-48.101	-4.655	-11.044	-280.884	-11.687	-171.934
6	2.0	49.0	49.0	-159.810	-47.833	-4.897	-11.011	-280.264	-11.799	-171.143
7	2.0	59.0	39.0	-158.494	-47.393	-5.520	-10.976	-278.689	-12.058	-169.204
8	2.0	69.0	29.0	-8.441	-5.797	-88.678	-11.230	-102.354	-53.476	-38.866
9	2.0	79.0	19.0	-13.094	-4.669	-91.499	-13.917	-98.158	-54.747	-41.265
10	2.0	89.0	9.0	-14.262	-4.408	-92.893	-14.824	-96.099	-55.133	-41.912
11	2.0	96.0	2.0	-14.758	-4.304	-94.684	-15.216	-93.431	-55.316	-42.199
12	10.0	2.0	88.0	-159.385	-49.776	-4.401	-11.107	-281.553	-11.242	-172.824
13	10.0	10.0	80.0	-159.187	-48.911	-4.476	-11.084	-281.352	-11.397	-172.551
14	10.0	20.0	70.0	-158.869	-48.469	-4.605	-11.054	-281.014	-11.517	-172.103
15	10.0	30.0	60.0	-158.399	-48.133	-4.808	-11.021	-280.491	-11.634	-171.430
16	10.0	40.0	50.0	-157.482	-47.743	-5.232	-10.987	-279.415	-11.818	-170.090
17	10.0	50.0	40.0	0.473	-8.143	-84.239	-10.947	-109.012	-51.125	-34.170
18	10.0	60.0	30.0	1.005	-7.909	-84.745	-10.907	-108.233	-51.279	-34.558
19	10.0	70.0	20.0	0.729	-7.678	-85.254	-10.864	-107.448	-51.423	-34.933
20	10.0	80.0	10.0	-10.706	-4.808	-91.640	-13.277	-97.891	-54.385	-40.764
21	10.0	88.0	2.0	-12.157	-4.476	-94.030	-14.397	-94.325	-54.342	-41.552
22	20.0	2.0	78.0	-159.098	-49.398	-4.638	-11.047	-280.930	-11.200	-171.992
23	20.0	10.0	70.0	-157.706	-48.682	-4.808	-11.021	-280.491	-11.388	-171.430
24	20.0	20.0	60.0	-156.789	-48.089	-5.232	-10.987	-279.415	-11.604	-170.090
25	20.0	30.0	50.0	1.442	-8.305	-84.343	-10.947	-108.857	-50.883	-33.687
26	20.0	40.0	40.0	2.248	-8.220	-84.817	-10.907	-108.125	-50.972	-33.936
27	20.0	50.0	30.0	2.672	-8.164	-85.129	-10.863	-107.635	-50.937	-33.960
28	20.0	60.0	20.0	3.053	-8.146	-85.475	-10.815	-107.092	-50.859	-33.900
29	20.0	70.0	10.0	3.532	-8.174	-86.008	-10.762	-106.266	-50.726	-33.739
30	22.0	76.0	2.0	15.974	-11.217	-92.826	-11.509	-96.413	-49.175	-29.447
31	18.0	80.0	2.0	-7.209	-5.458	-91.640	-11.365	-97.813	-53.425	-39.154
32	30.0	2.0	68.0	-156.027	-49.148	-5.403	-10.980	-278.984	-11.233	-169.563
33	30.0	10.0	60.0	3.266	-8.841	-85.041	-10.946	-107.809	-50.427	-32.773
34	30.0	20.0	50.0	15.526	-11.539	-91.200	-10.906	-98.550	-47.648	-28.456
35	30.0	30.0	40.0	16.172	-11.589	-91.587	-10.858	-97.946	-47.533	-28.521
36	30.0	40.0	30.0	16.156	-11.493	-91.669	-10.805	-97.796	-47.491	-28.393
37	30.0	50.0	20.0	16.132	-11.456	-91.800	-10.745	-97.569	-47.459	-28.229
38	30.0	60.0	10.0	16.106	-11.322	-92.066	-10.677	-97.137	-47.406	-27.997
39	30.0	68.0	2.0	16.084	-11.256	-92.797	-10.615	-96.009	-47.348	-27.644
40	40.0	10.0	50.0	16.663	-12.352	-91.701	-10.838	-97.765	-46.699	-28.628
41	40.0	20.0	40.0	16.407	-11.858	-91.629	-10.783	-97.845	-47.081	-28.429
42	40.0	30.0	30.0	16.309	-11.655	-91.661	-10.720	-97.766	-47.159	-28.264
43	40.0	40.0	20.0	16.243	-11.511	-91.759	-10.648	-97.583	-47.161	-28.068
44	40.0	50.0	10.0	16.189	-11.388	-91.995	-10.564	-97.187	-47.115	-27.798
45	40.0	58.0	2.0	16.156	-11.296	-92.701	-10.485	-96.089	-47.049	-27.386

TABLE 28b

300°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.8E-02	1.7E-01	2.6E-01	3.3E-01	7.2E-01	7.1E-01	0.
H2	4.2E-04	3.6E-04	4.3E-07	3.3E-01	4.0E-04	7.3E-07	4.0E-39
O2	0.	0.	0.	0.	0.	0.	5.0E-01
WATER	6.9E-01	3.3E-01	4.5E-07	3.3E-01	1.1E-01	4.8E-07	2.5E-01
CO	1.8E-09	6.0E-09	7.7E-06	1.6E-17	6.6E-09	4.5E-06	0.
CO2	2.7E-01	5.0E-01	7.3E-01	1.4E-12	1.7E-01	2.6E-01	2.5E-01
BENZENE	0.	3.2E-35	1.0E-07	0.	9.3E-32	3.4E-07	0.
NAPHTHALENE	0.	0.	4.6E-08	0.	0.	2.0E-07	0.
ASPHALT	0.	0.	4.8E-03	0.	0.	2.8E-02	0.
ACETYLENE	0.	1.2E-38	1.8E-29	0.	1.7E-37	2.7E-29	0.
ETHYLENE	1.2E-22	3.1E-21	5.3E-15	1.5E-26	4.8E-20	1.4E-14	0.
ETHANE	3.7E-12	8.1E-11	1.7E-07	3.5E-13	1.4E-09	7.3E-07	0.
FORMIC ACID	5.9E-16	9.4E-16	1.6E-18	2.4E-24	3.4E-16	1.0E-18	0.
ACETIC ACID	2.4E-15	1.9E-14	4.5E-14	1.1E-25	2.8E-14	4.3E-14	0.
FORMALDEHYDE	2.4E-21	6.9E-21	1.0E-20	1.6E-26	8.3E-21	1.0E-20	0.
ACETALDEHYDE	3.1E-24	4.4E-23	8.9E-20	2.3E-31	2.1E-22	1.4E-19	0.
METHANOL	3.9E-19	9.6E-19	1.7E-21	2.1E-21	1.3E-18	2.9E-21	0.
ETHANOL	2.5E-25	3.0E-24	7.2E-24	1.4E-29	1.6E-23	1.9E-23	0.
N2	1.6E-06	1.7E-06	1.9E-06	1.5E-08	2.2E-06	2.7E-06	1.3E-06
NH3	1.6E-09	1.3E-09	5.5E-14	3.4E-06	1.7E-09	1.5E-13	0.
HCN	5.1E-26	2.9E-25	1.2E-20	1.9E-30	1.3E-24	1.7E-20	0.
NO	0.	0.	0.	0.	0.	0.	6.6E-19
NO2	0.	0.	0.	0.	0.	0.	7.5E-15
N2O	0.	0.	0.	0.	0.	0.	8.5E-27
NITROUS ACID	0.	0.	0.	0.	0.	0.	3.0E-19
NITRIC ACID	0.	0.	0.	0.	0.	0.	4.7E-16
C2N2	0.	0.	0.	0.	0.	0.	0.
HNC	4.8E-35	1.5E-34	7.1E-33	0.	2.0E-34	6.5E-33	0.
FORMAMIDE	2.3E-36	6.3E-36	3.4E-37	0.	9.1E-36	5.3E-37	0.
GLYCINE	2.8E-36	2.2E-35	1.8E-36	0.	3.8E-35	2.8E-36	0.
ALANINE	0.	0.	0.	0.	0.	0.	0.
SERINE	0.	0.	0.	0.	0.	0.	0.
ASPARTIC ACID	0.	0.	0.	0.	0.	0.	0.
VALINE	0.	0.	0.	0.	0.	0.	0.
LEUCINE	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
OXAMIC ACID	0.	0.	0.	0.	0.	0.	0.
P2	0.	0.	0.	0.	0.	0.	0.
P406	7.8E-07	8.4E-07	9.3E-07	8.4E-07	1.1E-06	1.3E-06	0.
P4010	0.	0.	0.	0.	0.	0.	6.3E-07
PO	0.	0.	0.	0.	0.	0.	0.
PO2	0.	0.	0.	0.	0.	0.	0.
PH3	0.	0.	0.	0.	0.	0.	0.
PCl3	0.	0.	0.	0.	0.	0.	0.
POCl3	0.	0.	0.	0.	0.	0.	1.6E-37
PSCl3	0.	0.	3.5E-35	0.	0.	1.8E-34	0.
CL2	0.	0.	2.7E-38	0.	0.	3.3E-38	5.0E-07
HCl	3.1E-06	3.4E-06	3.7E-06	3.4E-06	4.5E-06	5.4E-06	1.5E-06
HOCl	0.	0.	0.	0.	0.	0.	2.8E-11
Cl2O	0.	0.	0.	0.	0.	0.	2.6E-25
CH3Cl	9.4E-19	5.1E-18	7.5E-15	1.1E-20	2.7E-17	1.7E-14	0.
CCl4	0.	0.	0.	0.	0.	0.	0.
COCl2	0.	0.	3.5E-35	0.	0.	2.5E-35	0.
S2	1.0E-26	1.7E-26	8.4E-22	2.0E-32	2.5E-26	2.4E-21	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	3.1E-06	3.4E-06	9.1E-07	3.4E-06	4.5E-06	2.6E-06	0.
S02	8.4E-26	3.3E-26	9.9E-30	4.3E-35	3.8E-27	6.4E-30	1.6E-16
S03	0.	0.	0.	0.	0.	0.	2.5E-06
COS	2.4E-12	9.9E-12	2.8E-06	2.8E-23	1.3E-11	2.8E-06	0.
CS2	4.4E-24	4.2E-23	2.3E-12	1.2E-34	2.2E-22	6.2E-12	0.
SULFUROUS ACID	0.	0.	0.	0.	0.	0.	0.
SULFURIC ACID	0.	0.	0.	0.	0.	0.	6.6E-19
METHANETHIOL	3.6E-17	2.0E-16	7.0E-14	4.3E-19	1.1E-15	3.2E-13	0.
DIMETHYLSULFIDE	5.2E-27	1.4E-25	6.7E-20	6.8E-31	3.0E-24	4.9E-19	0.
ETHANETHIOL	5.6E-25	1.5E-23	7.2E-18	7.3E-29	3.2E-22	5.3E-17	0.
DIETHYLSULFIDE	0.	0.	6.2E-28	0.	2.5E-37	1.2E-26	0.
OCTANETHIOL	0.	0.	0.	0.	0.	0.	0.
THIOFORMIC ACID	0.	0.	1.2E-38	0.	0.	2.0E-38	0.
THIOPACETIC ACID	0.	0.	0.	0.	0.	0.	0.
CYCLOPROP.THIOL	0.	0.	2.8E-28	0.	4.0E-38	1.9E-27	0.
CYCLOBUTA.THIOL	0.	0.	1.5E-33	0.	0.	1.6E-32	0.
CYCLOPENT.THIOL	0.	0.	9.6E-28	0.	0.	1.7E-26	0.
CYCLOHEXA.THIOL	0.	0.	3.4E-30	0.	0.	9.4E-29	0.
M.SULFONIC ACID	0.	0.	0.	0.	0.	0.	0.
E-SULFINIC ACID	5.2E-15	8.1E-14	4.3E-11	4.2E-22	5.1E-13	2.0E-10	0.
THIOPHENE	0.	3.6E-37	1.8E-16	0.	9.0E-35	6.7E-16	0.
BENZENETHIOL	0.	0.	2.8E-16	0.	0.	1.6E-15	0.
THIOLGLYCOL	0.	0.	0.	0.	0.	0.	0.
CYSTEINE	0.	0.	0.	0.	0.	0.	0.
METHIONINE	0.	0.	0.	0.	0.	0.	0.

TABLE 29a  
 300°K AND 0.2 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 25 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.  
 SYSTEMS CONTAINING LIQUID WATER HAVE BEEN OMITTED.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-161.300	-48.147	-0.837	-7.696	-288.757	-7.718	-176.694
2	2.0	9.0	89.0	-161.178	-47.355	-0.880	-7.678	-288.641	-7.726	-176.528
3	2.0	96.0	2.0	-21.666	-0.850	-94.684	-18.671	-91.704	-51.863	-42.200
4	10.0	2.0	88.0	-159.385	-48.049	-0.947	-7.653	-288.460	-7.676	-176.277
5	10.0	10.0	80.0	-159.187	-47.183	-1.022	-7.630	-288.260	-7.685	-176.004
6	10.0	88.0	2.0	-19.065	-1.022	-94.038	-17.852	-92.598	-51.389	-41.553
7	20.0	2.0	78.0	-158.098	-47.871	-1.184	-7.594	-287.837	-7.619	-175.446
8	20.0	10.0	70.0	-157.706	-46.955	-1.354	-7.568	-287.399	-7.633	-174.884
9	20.0	70.0	10.0	3.530	-6.447	-82.553	-7.309	-109.722	-45.547	-30.286
10	22.0	76.0	2.0	15.247	-9.309	-89.008	-8.055	-100.412	-44.175	-26.785
11	18.0	80.0	2.0	-14.117	-2.004	-91.640	-14.472	-96.086	-49.970	-39.155
12	30.0	2.0	68.0	-156.027	-47.421	-1.949	-7.526	-285.891	-7.565	-173.016
13	30.0	10.0	60.0	3.266	-7.114	-81.587	-7.493	-111.263	-45.247	-29.320
14	30.0	20.0	50.0	14.961	-9.671	-87.464	-7.453	-102.427	-42.609	-25.158
15	30.0	30.0	40.0	15.445	-9.680	-87.769	-7.405	-101.946	-42.503	-25.284
16	30.0	40.0	30.0	15.429	-9.584	-87.852	-7.351	-101.795	-42.492	-25.351
17	30.0	50.0	20.0	15.405	-9.497	-87.983	-7.291	-101.569	-42.459	-25.388
18	30.0	60.0	10.0	15.379	-9.414	-88.248	-7.223	-101.137	-42.406	-25.336
19	30.0	68.0	2.0	15.357	-9.348	-88.980	-7.161	-100.008	-42.348	-24.980
20	40.0	10.0	50.0	15.936	-10.444	-87.884	-7.385	-101.764	-41.702	-24.859
21	40.0	20.0	40.0	15.680	-9.949	-87.811	-7.329	-101.845	-42.085	-24.869
22	40.0	30.0	30.0	15.582	-9.746	-87.844	-7.266	-101.765	-42.160	-24.945
23	40.0	40.0	20.0	15.516	-9.602	-87.941	-7.194	-101.582	-42.161	-25.019
24	40.0	50.0	10.0	15.462	-9.480	-88.177	-7.111	-101.187	-42.115	-25.018
25	40.0	58.0	2.0	15.423	-9.387	-88.883	-7.032	-100.088	-42.051	-24.700

TABLE 29b

300°K AND 0.2 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH THREE SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS. SYSTEMS CONTAINING LIQUID WATER HAVE BEEN OMITTED.

COMPOUND	C	E	F
METHANE	7.2E-01	2.6E-01	7.1E-01
H2	1.3E-05	2.0E-08	3.3E-08
O2	0.	0.	0.
WATER	1.1E-01	9.4E-07	9.9E-07
CO	2.1E-10	1.7E-07	9.8E-08
CO2	1.7E-01	7.3E-01	2.6E-01
BENZENE	2.9E-30	1.2E-07	4.0E-07
NAPHTHALENE	0.	1.4E-07	5.9E-07
ASPHALT	0.	4.8E-03	2.8E-02
ACETYLENE	0.	1.9E-31	2.9E-31
ETHYLENE	4.8E-20	2.6E-15	6.6E-15
ETHANE	4.4E-08	3.7E-06	1.6E-05
FORMIC ACID	1.1E-14	7.4E-17	4.6E-17
ACETIC ACID	2.8E-11	4.5E-11	4.3E-11
FORMALDEHYDE	8.3E-21	1.0E-20	1.0E-20
ACETALDEHYDE	6.7E-21	2.0E-18	3.1E-18
METHANOL	4.0E-17	7.9E-20	1.3E-19
ETHANOL	1.6E-20	7.2E-21	1.9E-20
N2	2.2E-06	1.9E-06	2.7E-06
NH3	9.6E-09	5.3E-13	1.4E-12
HCN	2.2E-25	1.2E-21	1.8E-21
NO	0.	0.	0.
NO2	0.	0.	0.
N2O	0.	0.	0.
NITROUS ACID	0.	0.	0.
NITRIC ACID	0.	0.	0.
C2N2	0.	0.	0.
HNCO	1.1E-33	3.3E-32	3.0E-32
FORMAMIDE	1.6E-33	7.3E-35	1.1E-34
GLYCINE	6.7E-30	3.8E-31	5.9E-31
ALANINE	3.8E-35	5.0E-34	1.2E-33
SERINE	0.	0.	0.
ASPARTIC ACID	0.	0.	0.
VALINE	0.	0.	0.
LEUCINE	0.	0.	0.
FORMYLYGLYCINE	0.	0.	0.
OXAMIC ACID	0.	0.	0.
P2	0.	0.	0.
P406	1.1E-06	9.3E-07	1.3E-06
P4010	0.	0.	0.
PD	0.	0.	0.
PD2	0.	0.	0.
PH3	0.	0.	0.
PCL3	0.	0.	0.
POCL3	0.	0.	0.
PSCL3	0.	5.3E-32	1.5E-31
CL2	0.	6.0E-37	7.3E-37
HCl	4.5E-06	3.7E-06	5.4E-06
HOCl	0.	0.	0.
CL2O	0.	0.	0.
CH3CL	8.6E-16	1.6E-13	3.8E-13
CCL4	0.	0.	0.
COCL2	4.7E-38	1.7E-32	1.2E-32
S2	2.5E-26	5.5E-22	4.9E-22
S8	0.	0.	0.
H2S	4.5E-06	1.0E-06	1.7E-06
SO2	1.2E-25	5.2E-28	1.9E-28
SO3	0.	0.	0.
COS	1.3E-11	1.6E-06	8.7E-07
CS2	2.2E-22	7.3E-13	6.2E-13
SULFUROUS ACID	0.	0.	0.
SULFURIC ACID	0.	0.	0.
METHANETHIOL	3.3E-14	1.8E-12	4.6E-12
DIMETHYLSULFIDE	3.0E-21	3.7E-17	1.5E-16
ETHANETHIOL	3.2E-19	4.0E-15	1.7E-14
DIETHYLSULFIDE	2.5E-31	1.7E-22	1.8E-21
OCTANETHIOL	0.	3.9E-35	2.6E-33
THIOFORMIC ACID	0.	3.1E-37	2.9E-37
THIOACETIC ACID	0.	5.5E-37	8.2E-37
CYCLOPROP.THIOL	4.0E-35	7.5E-26	2.9E-25
CYCLOBUTA.THIOL	0.	8.8E-30	5.4E-29
CYCLOPENT.THIOL	1.2E-36	1.3E-22	1.2E-21
CYCLOHEXA.THIOL	0.	9.7E-24	1.5E-22
H.SULFONIC ACID	0.	0.	0.
E.SULFINIC ACID	1.6E-08	1.1E-06	2.8E-06
THIOPHENNE	2.8E-33	5.1E-16	1.1E-15
BENZENETHIOL	0.	8.7E-15	2.7E-14
THIOLYGLYCOL	0.	0.	0.
CYSTEINE	0.	0.	0.
METHIONINE	0.	0.	0.

TABLE 30a  
 300°K AND 20 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 13 SYSTEMS OF C, H, O, N, P,  
 S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.  
 SYSTEMS CONTAINING LIQUID WATER HAVE BEEN OMITTED.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	22.0	76.0	2.0	14.762	-8.036	-86.463	-5.753	-103.079	-40.843	-30.559
2	30.0	20.0	50.0	13.428	-8.136	-84.395	-5.150	-105.880	-39.537	-28.155
3	30.0	30.0	40.0	14.960	-8.407	-85.224	-5.102	-104.612	-39.170	-28.668
4	30.0	40.0	30.0	14.944	-8.312	-85.307	-5.049	-104.461	-39.161	-29.021
5	30.0	50.0	20.0	14.920	-8.225	-85.438	-4.989	-104.235	-39.126	-29.245
6	30.0	60.0	10.0	14.894	-8.141	-85.703	-4.921	-103.803	-39.074	-29.291
7	30.0	68.0	2.0	14.872	-8.075	-86.435	-4.859	-102.674	-39.016	-28.788
8	40.0	10.0	50.0	15.452	-9.171	-85.339	-5.082	-104.430	-38.368	-24.980
9	40.0	20.0	40.0	15.195	-8.677	-85.267	-5.027	-104.511	-38.751	-27.331
10	40.0	30.0	30.0	15.097	-8.474	-85.299	-4.964	-104.431	-38.829	-28.193
11	40.0	40.0	20.0	15.031	-8.330	-85.396	-4.892	-104.248	-38.828	-28.685
12	40.0	50.0	10.0	14.977	-8.207	-85.632	-4.808	-103.853	-38.783	-28.908
13	40.0	58.0	2.0	14.938	-8.115	-86.338	-4.729	-102.754	-38.718	-28.520

TABLE 30b  
 300°K AND 20 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN  
 MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N,  
 P, S, AND Cl WITH TWO SELECTED RELATIVE ABUNDANCE RATIOS OF  
 C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE  
 TOTAL NUMBER OF MOLES OF ALL ELEMENTS. SYSTEMS  
 CONTAINING LIQUID WATER HAVE BEEN OMITTED.

COMPOUND	C	F
METHANE	2.6E-01	7.1E-01
H2	2.5E-09	4.2E-09
O2	0.	0.
WATER	1.5E-06	1.6E-06
CO	1.3E-08	7.7E-09
CO2	7.3E-01	2.6E-01
BENZENE	1.4E-07	4.6E-07
NAPHTHALENE	2.8E-07	1.2E-06
ASPHALT	4.8E-03	2.8E-02
ACETYLENE	9.2E-33	1.4E-32
ETHYLENE	1.6E-15	4.0E-15
ETHANE	2.9E-05	1.3E-04
FORMIC ACID	9.5E-16	5.8E-16
ACETIC ACID	4.5E-09	4.3E-09
FORMALDEHYDE	1.0E-20	1.0E-20
ACETALDEHYDE	1.5E-17	2.4E-17
METHANOL	1.0E-18	1.7E-18
ETHANOL	7.2E-19	1.9E-18
N2	1.9E-06	2.7E-06
NH3	2.4E-12	6.5E-12
HCN	2.6E-22	3.9E-22
NO	0.	0.
NO2	0.	0.
N2O	0.	0.
NITROUS ACID	0.	0.
NITRIC ACID	0.	0.
C2N2	0.	0.
HNCO	9.3E-32	8.5E-32
FORMAMIDE	2.6E-33	4.0E-33
GLYCINE	1.4E-27	2.1E-27
ALANINE	1.4E-29	3.4E-29
SERINE	0.	0.
ASPARTIC ACID	2.6E-36	2.3E-36
VALINE	6.6E-34	4.1E-33
LEUCINE	3.1E-36	3.0E-35
FORMYLGLYCINE	0.	0.
OXAMIC ACID	2.7E-37	1.5E-37
P2	0.	0.
P4O6	9.3E-07	1.3E-06
P4O10	0.	0.
PO	0.	0.
PO2	0.	0.
PH3	0.	0.
PCL3	0.	0.
POCL3	5.9E-37	1.1E-36
PSCL3	2.7E-32	4.4E-32
CL2	4.7E-36	5.8E-36
HCL	3.7E-06	5.4E-06
HOCL	0.	0.
CL2O	0.	0.
CH3CL	1.3E-12	3.0E-12
CCL4	0.	0.
COCL2	1.0E-30	7.3E-31
S2	6.3E-27	1.8E-27
S8	0.	0.
H2S	4.5E-09	4.1E-09
SO2	2.9E-29	5.9E-30
SO3	0.	0.
COS	4.2E-09	1.3E-09
CS2	5.2E-18	1.4E-18
SULFUROUS ACID	0.	0.
SULFURIC ACID	0.	0.
METHANETHIOL	6.1E-14	8.9E-14
DIMETHYLSULFIDE	9.9E-18	2.3E-17
ETHANETHIOL	1.1E-15	2.5E-15
DIETHYLSULFIDE	2.8E-21	1.6E-20
OCTANETHIOL	2.4E-30	9.2E-29
THIOFORMIC ACID	1.0E-38	0.
THIOACETIC ACID	1.5E-37	1.2E-37
CYCLOPROP.THIOL	1.2E-26	2.7E-26
CYCLOBUTA.THIOL	1.1E-29	3.9E-29
CYCLOCOPEN.THIOL	1.3E-21	7.0E-21
CYCLOHEXA.THIOL	7.7E-22	6.8E-21
M.SULFONIC ACID	0.	0.
E.SULFINIC ACID	3.7E-06	5.4E-06
THIOPHENENE	4.0E-18	4.8E-18
BENZENETHIOL	3.3E-16	5.9E-16
THIOLGLYCOL	0.	0.
CYSTEINE	0.	0.
METHIONINE	0.	0.

TABLE 31a

500°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\bar{F}_i/RT$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-98.161	-30.413	-4.291	-11.150	-154.076	-14.479	-99.418
2	2.0	9.0	89.0	-98.038	-29.621	-4.333	-11.132	-153.960	-15.235	-99.253
3	2.0	19.0	79.0	-97.832	-29.183	-4.409	-11.104	-153.757	-15.618	-98.971
4	2.0	29.0	69.0	-97.572	-28.892	-4.510	-11.075	-153.490	-15.851	-98.610
5	2.0	39.0	59.0	-97.219	-28.640	-4.655	-11.044	-153.111	-16.041	-98.112
6	2.0	49.0	49.0	-96.670	-28.372	-4.897	-11.011	-152.491	-16.243	-97.321
7	2.0	59.0	39.0	-95.355	-27.933	-5.520	-10.976	-150.916	-16.610	-95.383
8	2.0	69.0	29.0	-3.048	-4.943	-51.720	-11.002	-57.391	-39.654	-26.958
9	2.0	79.0	19.0	-1.603	-4.595	-52.871	-11.047	-55.683	-40.083	-27.734
10	2.0	89.0	9.0	-1.889	-4.405	-53.998	-11.092	-54.013	-40.352	-28.195
11	2.0	96.0	2.0	-2.331	-4.304	-55.765	-11.134	-51.382	-40.530	-28.473
12	10.0	2.0	88.0	-96.245	-30.315	-4.401	-11.107	-153.780	-14.492	-99.002
13	10.0	10.0	80.0	-96.048	-29.450	-4.476	-11.084	-153.579	-15.311	-98.729
14	10.0	20.0	70.0	-95.729	-29.008	-4.605	-11.054	-153.242	-15.692	-98.281
15	10.0	30.0	60.0	-95.259	-28.672	-4.808	-11.021	-152.719	-15.964	-97.609
16	10.0	40.0	50.0	-94.343	-28.282	-5.232	-10.907	-151.642	-16.282	-96.269
17	10.0	50.0	40.0	-2.225	-5.248	-51.292	-10.983	-58.022	-39.309	-26.309
18	10.0	60.0	30.0	-0.004	-4.817	-52.532	-10.999	-56.170	-39.767	-27.197
19	10.0	70.0	20.0	0.512	-4.705	-53.025	-10.981	-55.421	-39.843	-27.386
20	10.0	80.0	10.0	0.643	-4.609	-53.613	-10.962	-54.529	-39.899	-27.538
21	10.0	88.0	2.0	0.249	-4.473	-55.178	-10.977	-52.188	-40.060	-27.834
22	20.0	2.0	78.0	-94.958	-30.137	-4.638	-10.047	-153.157	-14.551	-98.171
23	20.0	10.0	70.0	-94.566	-29.221	-4.808	-11.021	-152.719	-15.415	-97.609
24	20.0	20.0	60.0	-93.650	-28.628	-5.232	-10.987	-151.642	-15.936	-96.269
25	20.0	30.0	50.0	-0.472	-5.333	-51.821	-10.979	-57.226	-39.241	-26.180
26	20.0	40.0	40.0	1.367	-5.034	-52.811	-10.964	-55.735	-39.494	-26.698
27	20.0	50.0	30.0	2.098	-5.002	-53.266	-10.925	-55.032	-39.438	-26.604
28	20.0	60.0	20.0	2.789	-5.035	-53.748	-10.873	-54.283	-39.302	-26.515
29	20.0	70.0	10.0	3.814	-5.176	-54.525	-10.806	-53.086	-39.027	-26.099
30	22.0	76.0	2.0	10.376	-6.721	-59.047	-11.529	-46.664	-38.927	-24.827
31	18.0	80.0	2.0	3.341	-5.017	-55.175	-10.786	-52.100	-39.148	-26.378
32	30.0	2.0	68.0	-92.888	-29.687	-5.403	-10.980	-151.210	-14.863	-95.741
33	30.0	10.0	60.0	2.258	-5.651	-52.973	-10.964	-55.482	-38.869	-25.466
34	30.0	20.0	50.0	5.536	-5.975	-54.669	-10.925	-52.928	-38.463	-24.740
35	30.0	30.0	40.0	8.712	-6.634	-56.411	-10.911	-50.309	-37.775	-24.088
36	30.0	40.0	30.0	10.436	-6.987	-57.528	-10.903	-48.628	-37.407	-24.224
37	30.0	50.0	20.0	10.527	-6.930	-57.741	-10.831	-48.274	-37.321	-24.013
38	30.0	60.0	10.0	10.521	-6.845	-58.055	-10.738	-47.756	-37.220	-23.656
39	30.0	68.0	2.0	10.503	-6.765	-59.021	-10.638	-46.257	-37.099	-23.038
40	40.0	10.0	50.0	10.862	-7.563	-57.579	-10.987	-48.595	-36.999	-24.532
41	40.0	20.0	40.0	10.772	-7.330	-57.575	-10.917	-48.565	-37.034	-24.306
42	40.0	30.0	30.0	10.711	-7.172	-57.618	-10.840	-48.463	-37.097	-24.191
43	40.0	40.0	20.0	10.660	-7.040	-57.723	-10.749	-48.260	-37.046	-23.921
44	40.0	50.0	10.0	10.612	-6.916	-57.984	-10.637	-47.812	-36.947	-23.518
45	40.0	58.0	2.0	10.571	-6.807	-58.886	-10.513	-46.398	-36.808	-22.820

TABLE 31b

500°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	1.1E-03	9.5E-02	2.4E-01	2.5E-01	6.2E-01	6.4E-01	0.
H2	1.4E-01	2.1E-01	8.6E-03	5.0E-01	1.6E-01	5.7E-03	3.2E-22
O2	0.	0.	0.	0.	0.	0.	5.0E-01
WATER	5.8E-01	1.9E-01	2.2E-04	2.0E-01	2.6E-02	2.7E-05	2.5E-01
CO	5.2E-04	4.1E-03	1.7E-01	9.0E-04	8.6E-03	2.1E-01	2.4E-24
CO2	2.8E-01	5.0E-01	5.7E-01	4.8E-02	1.9E-01	1.3E-01	2.5E-01
BENZENE	1.2E-33	9.7E-24	9.0E-09	1.6E-24	9.8E-18	1.3E-24	0.
NAPHTHALENE	0.	1.3E-38	2.7E-12	0.	1.7E-28	3.6E-05	0.
ASPHALT	0.	0.	1.3E-18	0.	0.	1.9E-02	0.
ACETYLENE	3.7E-24	7.5E-21	7.3E-16	4.1E-21	7.5E-19	1.8E-14	0.
ETHYLENE	1.7E-16	5.3E-13	2.1E-09	6.8E-13	4.0E-11	3.4E-08	0.
ETHANE	3.8E-13	1.8E-09	2.9E-07	5.5E-09	1.0E-07	3.1E-06	0.
FORMIC ACID	1.7E-12	4.6E-12	2.2E-13	1.1E-12	1.3E-12	3.2E-14	3.5E-33
ACETIC ACID	5.5E-16	8.2E-14	2.4E-13	2.1E-14	2.0E-13	1.5E-13	0.
FORMALDEHYDE	7.3E-14	8.9E-13	1.5E-12	4.5E-13	1.4E-12	1.2E-12	0.
ACETALDEHYDE	5.4E-19	3.6E-16	4.0E-14	2.1E-16	5.0E-15	1.2E-13	0.
METHANOL	2.3E-15	4.2E-14	3.0E-15	5.5E-14	5.0E-14	1.5E-15	0.
ETHANOL	1.8E-22	1.9E-19	8.5E-19	2.6E-19	2.0E-18	1.7E-18	0.
N2	1.4E-06	1.5E-06	1.7E-06	1.5E-06	2.1E-06	2.4E-06	1.3E-06
NH3	4.0E-09	7.8E-09	6.8E-11	2.6E-08	6.0E-09	4.3E-11	0.
HCN	7.2E-17	3.3E-15	1.1E-12	2.5E-15	3.9E-14	6.4E-12	0.
NO	7.3E-33	1.6E-33	4.7E-35	7.3E-34	3.4E-34	1.1E-35	1.3E-12
NO2	0.	0.	0.	0.	0.	0.	1.5E-12
N2O	0.	0.	0.	0.	0.	0.	4.3E-21
NITROUS ACID	0.	0.	0.	0.	0.	0.	2.4E-16
NITRIC ACID	0.	0.	0.	0.	0.	0.	4.8E-17
C2N2	1.0E-38	1.4E-35	3.6E-29	3.2E-36	2.5E-33	1.9E-27	0.
HNCO	8.7E-17	8.8E-16	7.9E-15	2.9E-16	1.9E-15	9.0E-15	0.
FORMAMIDE	4.6E-28	7.1E-27	2.6E-27	5.0E-27	1.1E-26	2.0E-27	0.
GLYCINE	3.7E-33	7.0E-31	4.5E-31	2.6E-31	1.8E-30	2.6E-31	0.
ALANINE	0.	9.7E-38	3.9E-36	4.4E-38	2.1E-36	8.9E-36	0.
SERINE	0.	0.	0.	0.	0.	0.	0.
ASPARTIC ACID	0.	0.	0.	0.	0.	0.	0.
VALINE	0.	0.	0.	0.	0.	0.	0.
LEUCINE	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
OXAMIC ACID	1.7E-37	4.5E-36	1.9E-36	3.4E-37	2.7E-36	3.3E-37	0.
P2	0.	0.	0.	0.	0.	1.7E-38	0.
P4C6	7.2E-07	7.5E-07	8.4E-07	7.6E-07	1.0E-06	1.2E-06	0.
P4Cl0	0.	0.	0.	0.	0.	0.	6.3E-07
PO	6.0E-34	1.3E-33	8.1E-33	1.9E-33	3.3E-33	2.0E-32	0.
PO2	1.4E-29	6.7E-30	1.1E-30	4.0E-30	3.1E-30	5.4E-31	2.2E-30
PH3	3.4E-27	6.4E-26	1.2E-25	7.7E-25	5.9E-25	8.2E-25	0.
PCl3	0.	0.	2.9E-38	0.	0.	2.0E-36	0.
POCl3	0.	0.	4.5E-38	0.	0.	6.0E-37	1.7E-31
PSCl3	0.	0.	5.6E-36	0.	0.	5.8E-34	0.
Cl2	3.6E-31	2.5E-31	7.7E-30	1.1E-31	6.3E-31	2.3E-29	1.2E-19
HCl	2.9E-06	3.0E-06	3.4E-06	3.0E-06	4.1E-06	4.7E-06	2.5E-06
HuCl	2.6E-31	5.9E-32	1.8E-33	2.7E-32	1.5E-32	4.9E-34	4.2E-11
Cl2O	0.	0.	0.	0.	0.	0.	1.1E-23
CH3Cl	3.4E-17	2.0E-15	1.4E-13	2.3E-15	2.4E-14	7.9E-13	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
CCl2Cl2	7.0E-34	3.9E-33	5.0E-30	3.7E-34	2.0E-32	1.8E-29	1.1E-33
S2	7.0E-20	3.2E-20	6.0E-18	6.0E-21	1.1E-19	1.4E-17	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	2.9E-06	3.0E-06	1.7E-06	3.0E-06	4.1E-06	1.7E-06	0.
SO2	5.6E-19	1.8E-20	1.9E-22	1.0E-21	1.1E-21	1.1E-23	1.1E-09
SO3	6.8E-36	4.9E-36	0.	0.	0.	0.	2.5E-06
COS	9.4E-10	2.9E-09	1.7E-06	2.7E-10	1.1E-08	3.0E-06	0.
CS2	2.3E-19	3.8E-18	1.1E-12	3.9E-19	1.5E-16	1.6E-11	0.
SULFURIC ACID	0.	0.	0.	0.	0.	0.	2.3E-34
SULFURIC ACID	0.	0.	0.	0.	0.	0.	3.4E-18
METHANETHIOL	3.7E-16	2.1E-14	7.4E-13	2.4E-14	2.5E-13	3.0E-12	0.
DIMETHYLSULFIDE	9.5E-26	3.1E-22	6.8E-19	4.0E-22	3.2E-20	1.1E-17	0.
ETHANETHIOL	2.6E-24	8.2E-21	1.8E-17	1.1E-20	8.5E-19	2.9E-16	0.
DIETHYLSULFIDE	0.	4.1E-35	3.6E-28	6.9E-35	3.2E-31	9.4E-26	0.
OCTANETHIOL	0.	0.	0.	0.	0.	0.	0.
THIOFORMIC ACID	1.0E-29	8.5E-29	2.0E-27	1.9E-29	2.4E-28	2.4E-27	0.
THIOACETIC ACID	0.8E-36	4.1E-33	6.0E-30	1.0E-33	1.0E-31	2.9E-29	0.
CYCLOPROP.THIOL	0.2E-34	9.6E-29	3.3E-22	6.1E-29	1.2E-25	3.2E-20	0.
CYCLOBUTA.THIOL	0.	3.3E-36	7.2E-28	2.4E-36	3.5E-32	2.8E-25	0.
CYCLOPENT.THIOL	0.	5.8E-39	7.9E-29	4.7E-39	5.2E-34	1.2E-25	0.
CYCLOHEXA.THIOL	0.	0.	3.1E-31	0.	2.8E-37	2.0E-27	0.
M.SULFONIC ACID	0.	0.	0.	0.	0.	0.	0.
E.SULFINIC ACID	1.5E-22	1.1E-19	6.3E-18	6.1E-20	2.0E-18	2.0E-17	0.
THIOPHENE	4.0E-33	1.1E-26	1.9E-15	1.5E-27	2.1E-22	1.3E-12	0.
BENZENETHIOL	0.	5.9E-34	7.4E-18	4.2E-35	1.1E-27	1.7E-13	0.
THIODGLYCOL	0.	6.3E-38	3.8E-36	3.7E-38	1.2E-36	1.2E-35	0.
CYSTEINE	0.	0.	0.	0.	0.	0.	0.
METHIONINE	0.	0.	0.	0.	0.	0.	0.

TABLE 32a

500°K AND 0.2 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\bar{F}_j/RT$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-98.161	-28.686	-0.837	-7.696	-160.984	-9.295	-102.879
2	2.0	9.0	89.0	-98.038	-27.895	-0.880	-7.678	-160.867	-10.049	-102.714
3	2.0	19.0	79.0	-97.832	-27.456	-0.955	-7.650	-160.664	-10.433	-102.432
4	2.0	29.0	69.0	-97.572	-27.165	-1.056	-7.621	-160.398	-10.666	-102.068
5	2.0	39.0	59.0	-97.219	-26.913	-1.202	-7.590	-160.019	-10.856	-101.571
6	2.0	49.0	49.0	-96.670	-26.645	-1.443	-7.557	-159.398	-11.058	-100.780
7	2.0	59.0	39.0	-95.355	-26.206	-2.066	-7.522	-157.824	-11.427	-98.842
8	2.0	69.0	29.0	-93.222	-2.275	-49.899	-7.654	-58.368	-35.306	-25.277
9	2.0	79.0	19.0	-7.573	-1.215	-52.577	-9.675	-54.385	-36.506	-27.538
10	2.0	89.0	9.0	-8.742	-0.954	-53.971	-10.582	-52.326	-36.892	-28.184
11	2.0	96.0	2.0	-9.238	-0.850	-55.763	-10.974	-49.658	-37.077	-28.472
12	10.0	2.0	88.0	-96.245	-28.588	-0.947	-7.653	-160.687	-9.307	-102.463
13	10.0	10.0	80.0	-96.048	-27.723	-1.022	-7.630	-160.486	-10.126	-102.188
14	10.0	20.0	70.0	-95.729	-27.281	-1.151	-7.600	-160.149	-10.506	-101.740
15	10.0	30.0	60.0	-95.259	-26.945	-1.354	-7.568	-159.626	-10.778	-101.068
16	10.0	40.0	50.0	-94.343	-26.555	-1.778	-7.533	-158.550	-11.099	-99.728
17	10.0	50.0	40.0	-0.689	-3.039	-48.632	-7.512	-60.269	-34.543	-23.752
18	10.0	60.0	30.0	-0.119	-2.803	-49.150	-7.489	-59.473	-34.705	-24.145
19	10.0	70.0	20.0	-0.328	-2.589	-49.638	-7.474	-58.720	-34.835	-24.492
20	10.0	80.0	10.0	-5.186	-1.354	-52.719	-9.074	-54.118	-36.144	-27.037
21	10.0	88.0	2.0	-6.637	-1.022	-55.116	-10.155	-50.552	-36.600	-27.825
22	20.0	2.0	78.0	-94.958	-28.410	-1.184	-7.593	-160.064	-9.365	-101.630
23	20.0	10.0	70.0	-94.566	-27.494	-1.354	-7.568	-159.626	-10.229	-101.068
24	20.0	20.0	60.0	-93.650	-26.901	-1.778	-7.533	-158.550	-10.753	-99.728
25	20.0	30.0	50.0	0.292	-3.276	-48.744	-7.502	-60.100	-34.304	-23.275
26	20.0	40.0	40.0	1.119	-3.109	-49.229	-7.467	-59.353	-34.393	-23.533
27	20.0	50.0	30.0	1.553	-3.054	-49.546	-7.426	-58.857	-34.361	-23.555
28	20.0	60.0	20.0	1.945	-3.038	-49.896	-7.378	-58.308	-34.281	-23.490
29	20.0	70.0	10.0	2.447	-3.071	-50.437	-7.323	-57.469	-34.142	-23.318
30	22.0	76.0	2.0	9.663	-4.806	-54.661	-8.056	-51.506	-33.892	-21.660
31	18.0	80.0	2.0	-1.691	-2.003	-52.720	-7.590	-54.037	-35.184	-25.430
32	30.0	2.0	68.0	-92.888	-27.960	-1.949	-7.526	-158.118	-9.681	-99.200
33	30.0	10.0	60.0	2.135	-3.730	-49.452	-7.495	-59.038	-33.849	-22.364
34	30.0	20.0	50.0	7.022	-4.581	-51.927	-7.453	-55.305	-32.913	-20.580
35	30.0	30.0	40.0	9.859	-5.177	-53.414	-7.407	-53.053	-32.225	-20.785
36	30.0	40.0	30.0	9.845	-5.082	-53.497	-7.354	-52.900	-32.212	-20.652
37	30.0	50.0	20.0	9.822	-4.995	-53.629	-7.293	-52.673	-32.178	-20.482
38	30.0	60.0	10.0	9.796	-4.912	-53.895	-7.225	-52.239	-32.125	-20.239
39	30.0	68.0	2.0	9.774	-4.845	-54.633	-7.162	-51.101	-32.066	-19.858
40	40.0	10.0	50.0	10.344	-5.926	-53.527	-7.389	-52.874	-31.440	-20.866
41	40.0	20.0	40.0	10.096	-5.446	-53.458	-7.332	-52.949	-31.807	-20.708
42	40.0	30.0	30.0	9.999	-5.245	-53.490	-7.269	-52.869	-31.881	-20.532
43	40.0	40.0	20.0	9.933	-5.101	-53.588	-7.197	-52.686	-31.881	-20.329
44	40.0	50.0	10.0	9.880	-4.978	-53.824	-7.113	-52.289	-31.834	-20.048
45	40.0	58.0	2.0	9.840	-4.885	-54.535	-7.032	-51.183	-31.768	-19.607

TABLE 32b

500°K AND 0.2 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.5E-02	1.6E-01	2.6E-01	3.3E-01	7.2E-01	7.1E-01	0.
H2	1.1E-02	1.0E-02	1.6E-04	3.3E-01	1.1E-02	2.7E-04	1.0E-23
O2	0.	0.	0.	0.	0.	0.	5.0E-01
WATER	6.8E-01	3.3E-01	7.9E-05	3.3E-01	1.1E-01	8.3E-05	2.5E-01
CO	3.4E-05	1.2E-04	1.1E-02	6.4E-09	1.3E-04	6.4E-03	7.6E-26
CO2	2.7E-01	5.0E-01	7.2E-01	8.5E-07	1.7E-01	2.6E-01	2.5E-01
BENZENE	6.7E-27	2.3E-22	5.5E-05	3.2E-34	8.2E-19	1.9E-04	0.
NAPHTHALENE	0.	5.1E-36	3.0E-05	0.	4.1E-30	1.3E-04	0.
ASPHALT	0.	0.	4.5E-03	0.	0.	2.7E-02	0.
ACETYLENE	6.6E-24	2.1E-22	1.3E-16	2.4E-26	3.3E-21	2.0E-16	0.
ETHYLENE	2.5E-14	7.1E-13	7.1E-09	2.7E-15	1.2E-11	1.8E-08	0.
ETHANE	4.7E-09	1.1E-07	1.8E-05	1.4E-08	2.0E-06	7.9E-05	0.
FORMIC ACID	1.4E-10	2.2E-10	5.1E-12	1.2E-14	7.9E-11	3.1E-12	1.1E-31
ACETIC ACID	1.7E-11	1.4E-10	3.3E-10	5.0E-16	2.1E-10	3.2E-10	0.
FORMALDEHYDE	4.0E-13	1.2E-12	1.8E-12	2.2E-15	1.4E-12	1.7E-12	0.
ACETALDEHYDE	1.1E-15	1.8E-14	2.7E-12	2.0E-18	8.7E-14	4.2E-12	0.
METHANOL	1.0E-12	2.6E-12	6.4E-14	1.6E-13	3.4E-12	1.1E-13	0.
ETHANOL	3.2E-17	4.4E-16	1.1E-15	1.7E-18	2.3E-15	2.8E-15	0.
N2	1.5E-06	1.6E-06	1.8E-06	6.6E-08	2.2E-06	2.7E-06	1.3E-06
NH3	9.8E-08	8.3E-08	1.8E-10	3.2E-06	1.1E-07	4.7E-10	0.
HCN	9.9E-17	5.9E-16	4.9E-13	1.2E-18	2.7E-15	7.2E-13	0.
NO	3.4E-33	1.9E-33	3.1E-35	1.2E-35	6.7E-34	2.3E-35	1.3E-12
NO2	0.	0.	0.	0.	0.	0.	4.8E-11
N2O	0.	0.	0.	0.	0.	0.	1.4E-19
NITROUS ACID	0.	0.	0.	0.	0.	0.	4.2E-14
NITRIC ACID	0.	0.	0.	0.	0.	0.	2.7E-13
C2N2	2.2E-37	9.1E-36	4.0E-28	0.	1.7E-34	5.1E-28	0.
HNCO	1.7E-15	5.6E-15	7.1E-14	3.6E-19	7.5E-15	6.5E-14	0.
FORMAMIDE	7.5E-25	2.1E-24	4.3E-25	4.6E-27	3.1E-24	6.7E-25	0.
GLYCINE	3.3E-26	2.8E-25	8.6E-26	1.1E-30	4.9E-25	1.3E-25	0.
ALANINE	3.2E-32	1.4E-30	4.3E-29	3.4E-37	1.0E-29	1.1E-28	0.
SERINE	0.	0.	0.	0.	0.	0.	0.
ASPARTIC ACID	0.	0.	2.0E-37	0.	1.1E-38	1.8E-37	0.
VALINE	0.	0.	1.1E-35	0.	0.	6.7E-35	0.
LEUCINE	0.	0.	5.4E-39	0.	0.	5.4E-38	0.
FORMYLGLYCINE	0.	0.	6.3E-39	0.	0.	0.	0.
OXAMIC ACID	2.6E-31	1.4E-30	4.0E-31	5.0E-39	6.7E-31	2.2E-31	0.
P2	0.	0.	0.	0.	0.	0.	0.
P4O6	7.7E-07	8.4E-07	9.2E-07	8.4E-07	1.1E-06	1.3E-06	0.
P4O10	0.	0.	0.	0.	0.	0.	6.3E-07
PU	9.1E-37	1.3E-36	1.0E-35	7.2E-36	2.5E-36	1.4E-35	0.
PO2	3.1E-31	2.3E-31	2.9E-32	4.1E-32	1.4E-31	2.5E-32	2.2E-33
PH3	2.7E-28	5.5E-28	6.1E-28	2.0E-23	4.1E-27	3.0E-27	0.
PCl3	0.	0.	3.2E-35	0.	0.	9.6E-35	0.
POCl3	8.3E-38	1.8E-37	1.0E-33	5.4E-39	7.5E-37	1.9E-33	3.0E-29
PSCl3	6.0E-39	2.9E-38	1.7E-31	0.	5.0E-37	8.7E-31	0.
CL2	5.0E-30	6.7E-30	5.1E-28	2.0E-31	1.1E-29	6.2E-28	3.7E-09
HCl	3.1E-06	3.4E-06	3.7E-06	3.4E-06	4.5E-06	5.3E-06	2.5E-06
HOCl	4.0E-30	2.4E-30	4.0E-32	7.2E-32	9.4E-31	3.5E-32	1.3E-09
Cl2O	0.	0.	0.	0.	0.	0.	1.1E-20
CH3Cl	1.4E-14	8.1E-14	8.9E-12	5.0E-15	4.4E-13	2.0E-11	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
COCl2	6.4E-31	2.9E-30	2.1E-26	4.9E-36	5.4E-30	1.5E-26	1.1E-30
S2	1.2E-20	1.8E-20	4.4E-18	1.6E-23	2.8E-20	1.3E-17	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	3.1E-06	3.4E-06	8.4E-07	3.4E-06	4.5E-06	2.5E-06	0.
SO2	1.5E-18	5.6E-19	2.0E-21	1.6E-23	6.2E-20	1.3E-21	3.5E-11
SU3	2.6E-34	5.3E-35	0.	0.	1.8E-36	0.	2.5E-06
COS	4.6E-10	1.9E-09	2.9E-06	3.2E-15	2.7E-09	2.9E-06	0.
CS2	1.8E-19	1.7E-18	2.6E-12	2.8E-24	9.8E-18	7.2E-12	0.
SULFURCUS ACID	0.	0.	0.	0.	0.	0.	7.2E-33
SULFURIC ACID	0.	0.	0.	0.	0.	0.	3.4E-15
METHANETHIOL	1.5E-13	8.7E-13	2.2E-11	5.3E-14	4.7E-12	1.0E-10	0.
DIMETHYLSULFIDE	1.5E-20	4.6E-19	1.1E-15	1.7E-21	1.0E-17	8.5E-15	0.
ETHANETHIOL	4.1E-19	1.2E-17	3.1E-14	4.6E-20	2.7E-16	2.3E-13	0.
DIETHYLSULFIDE	9.7E-32	8.4E-29	2.1E-21	1.2E-33	3.0E-26	3.9E-20	0.
OCTANETHIOL	0.	0.	1.2E-34	0.	0.	1.5E-32	0.
THIOFORMIC ACID	7.3E-28	2.7E-27	6.3E-26	1.5E-31	4.0E-27	1.1E-25	0.
THIOPACETIC ACID	2.4E-31	4.7E-30	1.1E-26	1.6E-35	2.9E-29	3.0E-26	0.
CYCLOPROP.THIOL	6.1E-28	1.1E-25	1.7E-18	7.7E-31	9.4E-24	1.2E-17	0.
CYCLOBUTA.THIOL	1.4E-34	1.4E-31	2.2E-22	6.0E-38	4.9E-29	2.5E-21	0.
CYCLOCOPEN.THIOL	1.7E-36	9.1E-33	1.4E-21	0.	1.3E-29	2.5E-20	0.
CYCLOHEXA.THIOL	0.	2.1E-35	3.2E-22	0.	1.2E-31	9.1E-21	0.
M.SULFONIC ACID	3.4E-16	5.7E-15	2.1E-13	6.5E-19	3.7E-14	9.9E-13	0.
E-SULFINIC ACID	1.7E-28	2.2E-25	1.3E-12	8.2E-35	6.4E-23	5.1E-12	0.
THIOPHENC	7.7E-36	3.3E-31	1.2E-12	0.	1.5E-27	7.2E-12	0.
BENZENETHIOL	2.0E-34	3.4E-33	1.3E-31	3.9E-37	2.2E-32	6.0E-31	0.
THIOLYGLYCOL	0.	0.	9.3E-39	0.	0.	3.9E-38	0.
CYSTEINE	0.	0.	0.	0.	0.	0.	0.
METHIONINE	0.	0.	0.	0.	0.	0.	0.

TABLE 33a

500°K AND 20 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-98.161	-27.535	1.466	-5.393	-165.589	-6.117	-105.179
2	2.0	9.0	89.0	-98.038	-26.743	1.423	-5.375	-165.473	-6.681	-105.014
3	2.0	19.0	79.0	-97.832	-26.304	1.347	-5.348	-165.270	-6.996	-104.732
4	2.0	29.0	69.0	-97.572	-26.013	1.246	-5.319	-165.003	-7.218	-104.371
5	2.0	39.0	59.0	-97.219	-25.762	1.101	-5.288	-164.624	-7.402	-103.873
6	2.0	49.0	49.0	-96.670	-25.494	0.859	-5.255	-164.004	-7.604	-103.083
7	2.0	59.0	39.0	-95.355	-25.054	0.237	-5.220	-162.429	-7.973	-101.145
8	2.0	69.0	29.0	-7.526	-0.040	-49.757	-8.452	-57.429	-32.933	-25.138
9	2.0	79.0	19.0	-12.179	1.087	-52.577	-11.978	-53.234	-34.203	-27.536
10	2.0	89.0	9.0	-13.347	1.348	-53.971	-12.886	-51.174	-34.589	-28.183
11	2.0	96.0	2.0	-13.843	1.452	-55.763	-13.277	-48.507	-34.775	-28.471
12	10.0	2.0	88.0	-96.245	-27.437	1.356	-5.350	-165.293	-6.108	-104.763
13	10.0	10.0	80.0	-96.048	-26.572	1.280	-5.327	-165.092	-6.741	-104.490
14	10.0	20.0	70.0	-95.729	-26.130	1.151	-5.297	-164.754	-7.058	-104.043
15	10.0	30.0	60.0	-95.259	-25.794	0.949	-5.265	-164.231	-7.325	-103.370
16	10.0	40.0	50.0	-94.343	-25.404	0.525	-5.230	-163.155	-7.646	-102.031
17	10.0	50.0	40.0	-0.666	-1.874	-46.343	-5.244	-62.550	-31.093	-21.465
18	10.0	60.0	30.0	-0.131	-1.041	-46.850	-5.254	-61.770	-31.249	-21.854
19	10.0	70.0	20.0	-0.403	-1.411	-47.357	-5.303	-60.988	-31.391	-22.226
20	10.0	80.0	10.0	-9.791	0.949	-52.718	-11.338	-52.967	-33.841	-27.034
21	10.0	88.0	2.0	-11.243	1.280	-55.116	-12.458	-49.401	-34.298	-27.823
22	20.0	2.0	78.0	-94.958	-27.259	1.119	-5.291	-164.670	-6.126	-103.933
23	20.0	10.0	70.0	-94.566	-26.343	0.949	-5.265	-164.232	-6.782	-103.371
24	20.0	20.0	60.0	-93.650	-25.750	0.525	-5.230	-163.155	-7.299	-102.031
25	20.0	30.0	50.0	0.304	-2.116	-46.447	-5.216	-62.393	-30.851	-20.981
26	20.0	40.0	40.0	1.111	-1.951	-46.922	-5.191	-61.661	-30.938	-21.232
27	20.0	50.0	30.0	1.535	-1.895	-47.235	-5.152	-61.170	-30.905	-21.256
28	20.0	60.0	20.0	1.917	-1.877	-47.581	-5.105	-60.628	-30.827	-21.195
29	20.0	70.0	10.0	2.398	-1.905	-48.114	-5.046	-59.801	-30.694	-21.034
30	22.0	76.0	2.0	9.178	-3.534	-52.103	-5.753	-54.191	-30.558	-19.484
31	18.0	80.0	2.0	-6.294	0.209	-52.718	-9.078	-52.889	-32.881	-25.423
32	30.0	2.0	68.0	-92.888	-26.609	0.354	-5.223	-162.724	-6.343	-101.504
33	30.0	10.0	60.0	2.129	-2.372	-47.146	-5.196	-61.345	-30.395	-20.069
34	30.0	20.0	50.0	8.403	-3.774	-50.313	-5.150	-56.574	-29.114	-18.313
35	30.0	30.0	40.0	9.377	-3.905	-50.864	-5.102	-55.725	-28.886	-18.367
36	30.0	40.0	30.0	9.361	-3.810	-50.946	-5.049	-55.574	-28.875	-18.264
37	30.0	50.0	20.0	9.339	-3.722	-51.077	-4.909	-55.348	-28.842	-18.127
38	30.0	60.0	10.0	9.312	-3.639	-51.343	-4.921	-54.915	-28.789	-17.938
39	30.0	68.0	2.0	9.289	-3.573	-52.075	-4.858	-53.786	-28.732	-17.662
40	40.0	10.0	50.0	9.068	-4.663	-50.978	-5.083	-55.543	-28.084	-18.389
41	40.0	20.0	40.0	9.613	-4.175	-50.906	-5.027	-55.623	-28.466	-18.229
42	40.0	30.0	30.0	9.515	-3.972	-50.938	-4.904	-55.544	-28.543	-18.095
43	40.0	40.0	20.0	9.449	-3.828	-51.036	-4.892	-55.361	-28.544	-17.935
44	40.0	50.0	10.0	9.395	-3.705	-51.272	-4.808	-54.965	-28.498	-17.712
45	40.0	58.0	2.0	9.355	-3.613	-51.978	-4.729	-53.866	-28.433	-17.385

TABLE 33b

500°K AND 20 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.8E-02	1.7E-01	2.6E-01	3.3E-01	7.2E-01	7.1E-01	0.
H2	1.2E-03	1.0E-03	2.0E-05	3.3E-01	1.1E-03	3.5E-05	1.0E-24
O2	0.	0.	0.	0.	0.	0.	5.0E-01
WATER	6.9E-01	3.3E-01	1.3E-04	3.3E-01	1.1E-01	1.4E-04	2.5E-01
CO	3.5E-06	1.2E-05	8.7E-04	6.4E-13	1.3E-05	5.0E-24	7.6E-27
CO2	2.7E-01	5.0E-01	7.3E-01	8.0E-11	1.7E-01	2.6E-01	2.5E-01
BENZENE	8.3E-26	2.2E-21	6.3E-05	0.	6.7E-18	2.1E-04	0.
NAPHTHALENE	0.	5.0E-34	6.4E-05	0.	2.8E-28	2.8E-04	0.
ASPHALT	0.	0.	4.8E-03	0.	0.	2.8E-02	0.
ACETYLENE	7.1E-25	2.1E-23	6.5E-18	2.4E-30	3.1E-22	9.7E-18	0.
ETHYLENE	2.8E-14	7.2E-13	4.4E-09	2.7E-17	1.1E-11	1.1E-08	0.
ETHANE	3.3E-08	1.2E-06	1.4E-04	1.4E-08	2.0E-05	6.2E-04	0.
FORMIC ACID	1.4E-09	2.2E-09	6.5E-11	1.2E-16	8.1E-10	4.0E-11	1.1E-30
ACETIC ACID	1.3E-09	1.5E-08	3.3E-08	5.0E-18	2.1E-08	3.3E-08	0.
FORMALDEHYDE	4.1E-13	1.2E-12	1.8E-12	2.2E-17	1.4E-12	1.8E-12	0.
ACETALDEHYDE	1.2E-14	1.8E-13	2.1E-11	2.0E-20	8.5E-13	3.3E-11	0.
METHANOL	1.1E-11	2.7E-11	8.2E-13	1.0E-13	3.5E-11	1.4E-12	0.
ETHANOL	3.6E-15	4.5E-14	1.1E-13	1.7E-18	2.3E-13	2.9E-13	0.
N2	1.4E-06	1.5E-06	1.7E-06	7.1E-12	2.1E-06	2.7E-06	1.3E-06
NH3	3.1E-07	2.6E-07	8.1E-10	3.4E-06	3.5E-07	2.2E-09	7.4E-39
HCN	3.1E-17	1.8E-16	1.1E-13	1.3E-22	7.9E-16	1.6E-13	0.
NO	3.2E-33	1.9E-33	4.0E-35	1.2E-38	6.6E-34	3.0E-35	1.3E-12
NO2	0.	0.	0.	0.	0.	0.	4.8E-10
N2O	0.	0.	0.	0.	0.	0.	1.4E-18
NITROUS ACID	0.	0.	0.	0.	0.	0.	1.3E-12
NITRIC ACID	0.	0.	0.	0.	0.	0.	8.6E-11
C2N2	2.2E-37	8.4E-36	1.2E-28	0.	1.5E-34	1.9E-28	0.
HNCO	3.3E-15	1.7E-14	2.0E-13	3.7E-23	2.3E-14	1.8E-13	0.
FURMAMIDE	2.4E-23	6.7E-23	1.6E-23	4.8E-29	9.7E-23	2.4E-23	0.
GLYCINE	1.1E-22	8.8E-22	3.1E-22	1.2E-32	1.5E-21	4.8E-22	0.
ALANINE	1.1E-27	4.4E-26	1.2E-24	0.	3.1E-25	3.0E-24	0.
SERINE	2.1E-35	4.7E-34	2.5E-34	0.	1.0E-33	3.8E-34	0.
ASPARTIC ACID	1.9E-34	1.4E-32	5.9E-31	0.	3.3E-32	5.1E-31	0.
VALINE	1.1E-37	1.1E-34	1.9E-29	0.	1.2E-32	1.2E-28	0.
LEUCINE	0.	5.7E-39	7.6E-32	0.	2.5E-36	7.5E-31	0.
FORMYLGLYCINE	2.6E-37	6.7E-36	1.6E-34	0.	1.3E-35	1.6E-34	0.
OXAMIC ACID	8.3E-28	4.3E-27	1.5E-27	0.	2.1E-27	8.2E-28	0.
P2	0.	0.	0.	0.	0.	0.	0.
P4C6	7.8E-07	8.4E-07	9.3E-07	8.4E-07	1.1E-06	1.3E-06	0.
P4D10	1.2E-35	1.3E-36	0.	0.	1.5E-38	0.	6.3E-07
PO	9.2E-31	1.3E-38	9.2E-38	2.3E-37	2.4E-38	1.3E-37	0.
PO2	3.0E-32	2.3E-32	3.3E-33	1.3E-33	1.4E-32	2.9E-33	2.2E-35
PH3	9.2E-30	1.8E-29	1.9E-29	6.4E-22	1.3E-28	9.5E-29	0.
PCL3	0.	0.	4.9E-34	0.	3.7E-38	1.5E-33	0.
POCL3	2.6E-35	5.7E-35	2.0E-31	1.7E-37	2.3E-34	3.7E-31	9.4E-28
PSCL3	1.9E-36	9.2E-36	2.9E-29	2.7E-38	1.5E-34	1.3E-28	0.
CL2	4.9E-29	6.7E-29	4.1E-27	2.0E-31	1.1E-28	4.9E-27	3.7E-08
HCL	3.1E-06	3.4E-06	3.7E-06	3.4E-06	4.5E-06	5.4E-06	2.5E-06
HUCL	3.9E-29	2.4E-29	5.1E-31	7.2E-32	9.7E-30	4.6E-31	1.3E-08
CL20	0.	0.	0.	0.	0.	0.	1.1E-18
CH3CL	1.5E-13	8.2E-13	7.0E-11	5.0E-15	4.3E-12	1.6E-10	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
COCL2	6.4E-29	2.9E-28	1.3E-24	4.9E-36	5.2E-28	9.3E-25	1.1E-28
S2	1.1E-20	1.8E-20	5.6E-18	1.6E-25	2.7E-20	1.3E-17	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	3.1E-06	3.4E-06	1.2E-06	3.4E-06	4.5E-06	3.1E-06	0.
S02	1.4E-17	5.6E-18	3.7E-20	1.6E-25	6.3E-19	2.2E-20	3.5E-12
S03	2.4E-32	5.4E-33	7.0E-37	0.	1.8E-34	2.5E-37	2.5E-06
COS	4.6E-10	1.9E-09	2.5E-06	3.3E-19	2.6E-09	2.3E-06	0.
CS2	1.8E-19	1.7E-18	2.0E-12	2.6E-28	9.0E-18	4.4E-12	0.
SULFURUS ACID	8.1E-37	1.5E-37	0.	0.	0.	0.	7.2E-32
SULFURIC ACID	9.1E-39	0.	0.	0.	0.	0.	3.4E-13
METHANETHIOL	1.6E-12	3.8E-12	2.4E-10	5.3E-14	4.7E-11	1.0E-09	0.
DIMETHYLSULFIDE	1.7E-18	4.7E-17	1.0E-13	1.7E-21	9.9E-16	6.7E-13	0.
ETHANETHIOL	4.5E-17	1.3E-15	2.7E-12	4.7E-20	2.7E-14	1.8E-11	0.
DIETHYLSULFIDE	1.2E-27	8.6E-25	1.1E-17	1.2E-33	2.8E-22	1.9E-16	0.
OCTANETHIOL	0.	0.	2.5E-27	0.	4.2E-37	2.7E-25	0.
THIOFORMIC ACID	1.5E-27	2.7E-26	7.2E-25	1.5E-33	3.9E-26	1.1E-24	0.
THIODACETIC ACID	2.6E-29	4.7E-29	9.8E-25	1.6E-37	2.8E-27	2.4E-24	0.
CYCLOPROP.THIOL	6.9E-26	1.1E-23	9.5E-17	7.7E-33	8.7E-22	5.9E-16	0.
CYCLOBUTA.THIOL	1.7E-31	1.5E-26	9.5E-20	0.	4.4E-26	9.4E-19	0.
CYCLOPENT.THIOL	2.2E-32	9.4E-29	4.8E-18	0.	1.1E-25	7.5E-17	0.
CYCLOHEXA.THIOL	9.9E-35	2.1E-30	8.5E-18	0.	1.0E-26	2.1E-16	0.
M-SULFONIC ACID	5.3E-36	5.1E-36	0.	0.	7.6E-37	0.	0.
E-SULFINIC ACID	3.7E-13	5.8E-12	2.4E-10	6.0E-19	3.7E-11	1.0E-09	0.
THIOPHENE	1.9E-27	2.2E-24	3.5E-12	0.	5.4E-22	1.2E-11	0.
BENZENETHIOL	9.4E-34	3.2E-29	1.0E-11	0.	1.2E-25	8.1E-11	0.
THIOLGLYCOL	2.2E-31	3.5E-30	1.5E-28	3.9E-37	2.2E-29	6.0E-28	0.
CYSTEINE	1.2E-37	6.1F-36	3.0E-33	0.	5.2E-35	1.1E-32	0.
METHIONINE	0.	0.	0.	0.	0.	4.0E-38	0.

TABLE 34a

700°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F_j}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-71.087	-22.005	-4.291	-11.150	-99.421	-16.504	-68.030
2	2.0	9.0	89.0	-70.964	-21.213	-4.333	-11.131	-99.304	-17.259	-67.874
3	2.0	19.0	79.0	-70.758	-20.774	-4.409	-11.104	-99.101	-17.643	-67.609
4	2.0	29.0	69.0	-70.498	-20.483	-4.510	-11.075	-98.834	-17.876	-67.272
5	2.0	39.0	59.0	-70.145	-20.231	-4.655	-11.044	-98.456	-18.066	-66.812
6	2.0	49.0	49.0	-69.596	-19.963	-4.897	-11.011	-97.835	-18.268	-66.094
7	2.0	59.0	39.0	-68.281	-19.524	-5.520	-10.976	-96.261	-18.635	-64.405
8	2.0	69.0	29.0	-6.581	-4.936	-34.922	-11.003	-39.674	-33.293	-21.095
9	2.0	79.0	19.0	-6.955	-4.528	-36.360	-11.068	-37.549	-33.821	-22.038
10	2.0	89.0	9.0	-4.598	-4.351	-37.790	-11.124	-35.433	-34.112	-22.508
11	2.0	96.0	2.0	0.442	-4.280	-42.124	-11.158	-28.948	-34.248	-22.716
12	10.0	2.0	88.0	-69.171	-21.907	-4.401	-11.107	-99.124	-16.516	-67.638
13	10.0	10.0	80.0	-68.974	-21.041	-4.476	-11.034	-98.923	-17.335	-67.393
14	10.0	20.0	70.0	-68.655	-20.600	-4.605	-11.053	-98.586	-17.716	-66.968
15	10.0	30.0	60.0	-68.185	-20.263	-4.808	-11.021	-98.063	-17.988	-66.354
16	10.0	40.0	50.0	-67.269	-19.873	-5.232	-10.987	-96.987	-18.310	-65.164
17	10.0	50.0	40.0	-8.858	-5.258	-34.450	-10.984	-40.371	-32.921	-20.413
18	10.0	60.0	30.0	-5.282	-4.045	-36.374	-11.051	-37.518	-33.667	-21.773
19	10.0	70.0	20.0	-2.868	-4.451	-37.846	-11.109	-35.341	-33.979	-22.277
20	10.0	80.0	10.0	1.783	-4.373	-41.821	-11.154	-29.400	-34.148	-17.617
21	10.0	88.0	2.0	5.377	-4.411	-46.706	-11.024	-22.008	-33.848	-22.184
22	20.0	2.0	78.0	-67.884	-21.728	-4.638	-11.047	-98.501	-16.575	-66.866
23	20.0	15.0	75.0	-67.492	-20.613	-4.808	-11.021	-98.063	-17.439	-66.354
24	20.0	20.0	60.0	-66.576	-20.220	-5.232	-10.987	-96.987	-17.963	-65.164
25	20.0	30.0	50.0	-7.184	-5.322	-34.949	-10.983	-39.623	-32.857	-20.284
26	20.0	40.0	40.0	-3.465	-4.749	-36.998	-11.050	-36.583	-33.563	-21.562
27	20.0	50.0	30.0	-1.265	-4.590	-36.458	-11.108	-34.421	-33.840	-21.998
28	20.0	60.0	20.0	2.680	-4.521	-42.005	-11.152	-29.123	-33.995	-22.221
29	20.0	70.0	10.0	6.766	-4.082	-46.403	-10.982	-22.443	-33.496	-21.561
30	22.0	76.0	2.0	8.050	-4.825	-48.936	-11.621	-18.958	-34.613	-22.545
31	18.0	80.0	2.0	7.923	-4.794	-48.891	-10.846	-18.640	-33.133	-16.066
32	30.0	2.0	68.0	-65.814	-21.278	-5.403	-10.980	-96.555	-16.890	-64.709
33	30.0	10.0	60.0	-5.191	-5.613	-35.768	-10.982	-38.395	-32.564	-19.700
34	30.0	20.0	50.0	-2.008	-5.034	-37.622	-11.049	-35.648	-33.278	-20.991
35	30.0	30.0	40.0	-0.263	-4.832	-38.897	-11.108	-33.764	-33.596	-21.514
36	30.0	40.0	30.0	3.475	-4.731	-42.381	-11.152	-28.560	-33.785	-21.850
37	30.0	50.0	20.0	8.091	-5.057	-47.064	-10.997	-21.458	-33.150	-20.922
38	30.0	60.0	10.0	8.143	-4.960	-47.539	-10.865	-20.678	-32.979	-20.810
39	30.0	68.0	2.0	8.122	-4.853	-48.841	-10.722	-18.654	-32.798	-20.694
40	40.0	10.0	50.0	0.433	-5.375	-39.217	-11.108	-33.285	-33.056	-18.779
41	40.0	20.0	40.0	4.461	-5.087	-43.971	-11.155	-27.527	-33.437	-19.047
42	40.0	30.0	30.0	8.291	-5.305	-49.949	-11.045	-21.654	-32.992	-18.774
43	40.0	40.0	20.0	8.275	-5.178	-47.103	-10.928	-21.363	-32.886	-20.452
44	40.0	50.0	10.0	8.232	-5.034	-47.442	-10.772	-20.778	-32.718	-20.492
45	40.0	58.0	2.0	8.183	-4.893	-48.649	-10.595	-18.878	-32.505	-20.361

TABLE 34b

700°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	4.7E-09	7.9E-06	1.4E-04	6.7E-03	2.9E-01	3.7E-01	0.
H2	1.4E-01	3.7E-01	3.2E-01	8.0E-01	4.3E-01	2.5E-01	6.4E-15
O2	6.0E-27	3.7E-29	8.2E-31	2.4E-33	2.5E-37	2.6E-38	5.0E-01
WATER	5.0E-01	1.3E-01	1.6E-02	2.1E-03	1.2E-05	2.2E-06	2.5E-01
CO	7.3E-03	1.3E-01	4.6E-01	1.9E-01	2.9E-01	3.6E-01	7.1E-16
CO2	2.8E-01	3.7E-01	2.1E-01	4.6E-03	7.0E-05	2.9E-05	2.5E-01
BENZENE	0.	1.7E-33	2.3E-25	7.8E-19	1.2E-06	8.6E-04	0.
NAPHTHALENE	0.	0.	0.	7.9E-30	2.9E-09	3.0E-04	0.
ASPHALT	0.	0.	0.	0.	3.0E-14	1.6E-02	0.
ACETYLENE	3.5E-23	4.6E-18	2.4E-15	3.0E-13	4.1E-09	3.7E-08	0.
ETHYLENE	6.1E-21	2.3E-13	9.8E-13	3.7E-10	2.3E-06	1.2E-05	0.
ETHANE	8.0E-22	8.1E-10	3.0E-13	2.8E-10	9.3E-07	2.8E-06	0.
FORMIC ACID	3.4E-12	1.3E-11	6.0E-12	3.3E-13	2.8E-15	6.5E-16	1.5E-25
ACETIC ACID	7.3E-21	1.7E-17	1.6E-16	1.7E-16	1.1E-16	6.0E-17	0.
FORMALDEHYDE	4.8E-13	2.3E-11	7.2E-11	7.5E-11	6.0E-11	4.4E-11	0.
ACETALDEHYDE	1.1E-22	3.3E-18	2.2E-16	4.3E-15	2.7E-13	4.6E-13	0.
METHANOL	4.1E-17	5.3E-15	1.4E-14	3.7E-14	1.6E-14	6.7E-15	0.
ETHANOL	2.9E-26	2.3E-23	1.3E-21	6.4E-20	2.2E-18	2.1E-18	0.
N2	1.4E-06	1.3E-06	1.1E-06	1.0E-06	1.4E-06	1.8E-06	1.3E-06
NH3	1.1E-10	4.8E-19	3.5E-10	1.3E-09	6.2E-10	3.1E-10	1.1E-30
HCN	7.2E-16	2.5E-13	5.2E-12	6.1E-11	7.8E-09	2.6E-08	0.
NO	7.6E-23	5.6E-24	7.8E-25	4.0E-26	4.9E-28	1.8E-28	6.5E-10
NO2	1.8E-37	0.	0.	0.	0.	0.	1.4E-11
N2C	1.5E-31	1.0E-32	1.4E-33	6.6E-35	9.6E-37	3.9E-37	1.2E-18
NITROUS ACID	2.4E-34	2.3E-36	4.5E-38	0.	0.	0.	4.1E-15
NITRIC ACID	0.	0.	0.	0.	0.	0.	1.8E-17
C2N2	3.4E-35	1.4E-30	7.7E-28	4.2E-26	1.3E-21	2.5E-20	0.
HNC	6.9E-16	1.9E-14	5.9E-14	3.7E-14	4.8E-14	5.2E-14	1.4E-35
FORMAMIDE	1.7E-26	1.3E-24	3.5E-24	5.5E-24	3.8E-24	2.4E-24	0.
GLYCINE	3.9E-37	1.4E-33	1.1E-32	1.9E-32	1.1E-32	4.8E-33	0.
ALANINE	0.	0.	0.	0.	0.	0.	0.
SERINE	0.	0.	0.	0.	9.9E-38	1.0E-37	0.
ASPARTIC ACID	0.	0.	0.	0.	0.	0.	0.
VALINE	0.	0.	0.	0.	0.	0.	0.
LEUCINE	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
OXAMIC ACID	0.5E-37	5.5E-35	8.2E-35	2.9E-36	3.1E-38	7.8E-39	0.
P2	4.3E-32	8.4E-29	2.4E-26	1.5E-22	1.6E-16	5.5E-15	0.
P4O6	7.2E-07	6.3E-07	5.6E-07	5.1E-07	7.2E-07	9.2E-07	3.2E-33
P4Cl10	2.1E-35	0.	0.	0.	0.	0.	6.3E-07
P0	8.2E-22	2.8E-21	7.1E-21	3.0E-20	3.2E-19	6.0E-19	3.9E-34
P02	8.0E-19	2.2E-19	8.1E-20	1.6E-20	2.0E-21	1.2E-21	3.5E-18
PH3	1.1E-21	2.3E-19	3.0E-18	9.5E-16	3.9E-13	1.0E-12	0.
PCL3	4.8E-38	3.1E-37	4.7E-36	7.1E-35	5.2E-31	1.4E-29	0.
POCL3	1.1E-36	5.5E-37	1.2E-36	1.0E-36	7.6E-35	6.8E-34	3.4E-29
PSCL3	4.3E-39	8.7E-39	1.4E-37	1.0E-34	1.5E-32	8.6E-31	0.
CL2	1.3E-25	3.5E-26	3.3E-26	1.1E-26	4.0E-26	1.1E-25	2.0E-12
HCL	2.9E-06	2.5E-06	2.3E-06	2.1E-06	2.9E-06	3.7E-06	2.5E-06
HOC1	4.9E-24	3.4E-25	4.5E-26	2.2E-27	3.2E-29	1.3E-29	3.9E-11
CL2O	0.	0.	0.	0.	0.	0.	3.5E-23
CH3CL	4.3E-20	2.3E-17	4.3E-16	7.5E-15	8.3E-13	2.4E-12	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
CCCL2	1.8E-30	8.8E-30	3.0E-29	4.2E-30	2.3E-29	8.2E-29	2.9E-30
S2	9.3E-15	9.3E-16	1.0E-15	2.5E-12	9.4E-16	4.2E-15	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	2.9E-06	2.5E-06	2.3E-06	2.6E-04	2.9E-06	3.5E-06	0.
SO2	1.3E-12	2.6E-15	6.1E-17	8.0E-18	1.7E-23	3.8E-24	6.7E-07
SU3	4.0E-25	6.1E-29	2.1E-31	1.6E-33	0.	0.	1.8E-06
COS	4.8E-09	2.6E-08	1.0E-07	2.1E-06	6.0E-08	1.6E-07	0.
CS2	1.9E-17	4.1E-16	1.1E-14	2.1E-10	1.1E-11	2.0E-10	0.
SULFURCUS ACID	0.8E-33	2.4E-36	7.3E-39	0.	0.	0.	1.3E-27
SULFURIC ACID	4.1E-36	0.	0.	0.	0.	0.	8.3E-18
METHANETHIOL	2.5E-19	1.3E-16	2.4E-15	5.8E-12	4.8E-12	1.3E-11	0.
DIMETHYLSULFIDE	2.5E-32	7.9E-27	3.1E-24	1.4E-19	9.1E-18	5.8E-17	0.
ETHANETHIOL	3.7E-31	1.2E-25	4.6E-23	2.1E-18	1.4E-16	6.7E-16	0.
DIETHYLSULFIDE	0.	0.	0.	1.7E-32	6.7E-27	2.2E-25	0.
OCTANEETHIOL	0.	0.	0.	0.	0.	0.	0.
THIOFORMIC ACID	9.6E-26	1.4E-24	4.7E-24	2.4E-22	3.8E-24	5.8E-24	0.
THIOACETIC ACID	9.2E-37	8.4E-33	5.7E-31	5.1E-28	7.0E-28	2.5E-27	0.
CYCLOPROP.THIOL	0.	8.2E-32	7.8E-28	2.8E-22	2.6E-18	6.6E-17	0.
CYCLOBUTA.THIOL	0.	0.	1.3E-36	1.1E-29	7.8E-24	4.4E-22	0.
CYCLOPENT.THIOL	0.	0.	0.	3.3E-35	1.9E-27	2.5E-25	0.
CYCLODOXA.THIOL	0.	0.	0.	4.9E-39	2.3E-29	6.6E-27	0.
M.SULFONIC ACID	0.	0.	0.	0.	0.	0.	0.
F.SULFINIC ACID	1.5E-31	3.9E-27	2.2E-25	5.6E-22	3.7E-22	7.4E-22	0.
THIOPHEN	0.	4.8E-31	1.3E-25	1.0E-19	3.7E-13	6.4E-11	0.
BENZENETHIOL	0.	0.	2.5E-34	4.2E-26	1.2E-15	1.9E-12	0.
THIOLLYCOL	0.	6.8E-39	3.9E-37	9.8E-34	6.5E-34	1.3E-33	0.
CYSTEINE	0.	0.	0.	0.	0.	0.	0.
METHIONINE	0.	0.	0.	0.	0.	0.	0.

TABLE 35a

700°K AND 0.2 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NU.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-71.087	-20.278	-0.837	-7.696	-106.328	-11.322	-71.241
2	2.0	9.0	89.0	-70.964	-19.486	-0.880	-7.678	-106.212	-12.077	-71.075
3	2.0	19.0	79.0	-70.758	-19.047	-0.955	-7.650	-106.009	-12.461	-70.794
4	2.0	29.0	69.0	-70.498	-18.756	-1.056	-7.621	-105.742	-12.694	-70.433
5	2.0	39.0	59.0	-70.145	-18.504	-1.202	-7.590	-105.363	-12.884	-69.935
6	2.0	49.0	49.0	-69.596	-18.237	-1.443	-7.557	-104.743	-13.086	-69.144
7	2.0	59.0	39.0	-68.280	-17.797	-2.066	-7.522	-103.168	-13.455	-67.206
8	2.0	69.0	29.0	-2.958	-1.519	-34.823	-7.590	-38.092	-29.782	-21.013
9	2.0	79.0	19.0	-2.307	-1.176	-35.908	-7.709	-36.481	-30.189	-21.764
10	2.0	89.0	9.0	-3.058	-0.954	-37.161	-7.897	-34.626	-30.513	-22.311
11	2.0	96.0	2.0	-3.538	-0.850	-38.947	-8.044	-31.968	-30.694	-22.597
12	10.0	2.0	88.0	-69.171	-20.180	-0.947	-7.653	-106.032	-11.334	-70.825
13	10.0	10.0	80.0	-68.974	-19.314	-1.022	-7.630	-105.831	-12.153	-70.552
14	10.0	20.0	70.0	-68.655	-18.873	-1.151	-7.600	-105.493	-12.534	-70.104
15	10.0	30.0	60.0	-68.185	-18.536	-1.354	-7.567	-104.970	-12.806	-69.432
16	10.0	40.0	50.0	-67.269	-18.146	-1.778	-7.533	-103.894	-13.128	-68.092
17	10.0	50.0	40.0	-2.157	-1.847	-34.348	-7.544	-38.796	-29.417	-20.323
18	10.0	60.0	30.0	-0.480	-1.477	-35.352	-7.577	-37.289	-29.786	-21.061
19	10.0	70.0	20.0	-0.127	-1.352	-35.814	-7.577	-36.585	-29.868	-21.268
20	10.0	80.0	10.0	-0.219	-1.216	-36.465	-7.594	-35.600	-29.969	-21.503
21	10.0	88.0	2.0	-0.946	-1.021	-38.322	-7.713	-32.830	-30.222	-21.953
22	20.0	2.0	78.0	-67.884	-20.002	-1.184	-7.593	-105.409	-11.393	-69.994
23	20.0	10.0	70.0	-67.492	-19.086	-1.354	-7.567	-104.970	-12.257	-69.432
24	20.0	20.0	60.0	-66.576	-18.493	-1.778	-7.533	-103.894	-12.781	-68.092
25	20.0	30.0	50.0	-0.784	-1.975	-34.689	-7.534	-38.282	-29.280	-20.056
26	20.0	40.0	40.0	0.732	-1.709	-35.536	-7.530	-37.003	-29.512	-20.553
27	20.0	50.0	30.0	1.343	-1.658	-35.947	-7.496	-36.368	-29.490	-20.582
28	20.0	60.0	20.0	1.891	-1.662	-36.379	-7.447	-35.697	-29.393	-20.481
29	20.0	70.0	10.0	2.634	-1.739	-37.056	-7.382	-34.652	-29.199	-20.212
30	22.0	76.0	2.0	7.185	-2.778	-41.106	-8.085	-28.937	-29.602	-19.702
31	18.0	80.0	2.0	2.218	-1.585	-37.859	-7.364	-33.433	-29.294	-20.459
32	30.0	2.0	68.0	-65.814	-19.551	-1.949	-7.526	-103.463	-11.708	-67.564
33	30.0	10.0	60.0	1.028	-2.335	-35.405	-7.521	-37.206	-28.914	-19.328
34	30.0	20.0	50.0	2.873	-2.232	-36.418	-7.500	-35.678	-28.982	-19.499
35	30.0	30.0	40.0	4.254	-2.403	-37.243	-7.478	-34.430	-28.767	-19.115
36	30.0	40.0	30.0	5.711	-2.670	-38.228	-7.465	-32.945	-28.473	-18.926
37	30.0	50.0	20.0	7.272	-2.989	-39.524	-7.441	-30.990	-28.106	-18.616
38	30.0	60.0	10.0	7.336	-2.916	-39.934	-7.326	-30.316	-27.946	-18.302
39	30.0	68.0	2.0	7.325	-2.826	-41.088	-7.193	-28.519	-27.771	-17.860
40	40.0	10.0	50.0	6.867	-3.375	-38.809	-7.599	-32.141	-28.035	-18.604
41	40.0	20.0	40.0	7.509	-3.359	-39.371	-7.566	-31.282	-27.987	-18.874
42	40.0	30.0	30.0	7.508	-3.239	-39.455	-7.480	-31.113	-27.935	-18.697
43	40.0	40.0	20.0	7.477	-3.119	-39.576	-7.373	-30.878	-27.837	-18.460
44	40.0	50.0	10.0	7.437	-2.992	-39.867	-7.233	-30.371	-27.683	-18.107
45	40.0	58.0	2.0	7.395	-2.870	-40.930	-7.071	-28.696	-27.483	-17.584

TABLE 35b

700°K AND 0.2 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.2E-03	1.0E-01	2.1E-01	2.8E-01	6.0E-01	5.9E-01	0.
H2	1.2E-01	1.6E-01	4.1E-02	4.4E-01	1.5E-01	1.5E-02	2.0E-16
O2	7.3E-30	6.8E-31	2.2E-32	1.1E-31	3.3E-32	1.0E-34	5.0E-01
WATER	5.9E-01	2.4E-01	1.1E-02	2.5E-01	4.9E-02	2.6E-04	2.5E-01
CO	6.6E-03	3.6E-02	2.2E-01	5.5E-03	5.3E-02	3.3E-01	2.3E-17
CO2	2.8E-01	4.6E-01	5.2E-01	2.8E-02	1.5E-01	5.2E-02	2.5E-01
BENZENE	1.6E-25	1.2E-17	2.9E-10	8.0E-19	9.4E-13	1.4E-03	0.
NAPHTHALENE	0.	3.9E-28	3.0E-15	1.5E-30	5.5E-20	1.2E-03	0.
ASPHALT	0.	0.	2.3E-29	0.	0.	1.4E-02	0.
ACETYLENE	2.1E-17	8.9E-15	2.6E-12	3.6E-15	3.8E-13	4.4E-10	0.
ETHYLENE	3.4E-12	1.9E-09	1.4E-07	2.1E-09	7.6E-08	8.3E-06	0.
ETHANE	4.1E-10	3.0E-07	5.3E-06	8.6E-07	1.1E-05	1.2E-04	0.
FORMIC ACID	3.2E-09	6.9E-09	1.9E-09	1.1E-09	2.1E-09	6.9E-11	4.6E-24
ACETIC ACID	5.0E-12	2.6E-10	6.1E-10	4.3E-11	5.0E-10	1.7E-10	0.
FORMALDEHYDE	4.0E-10	2.9E-09	4.4E-09	1.2E-09	4.0E-09	2.3E-09	0.
ACETALCHYDYE	7.1E-14	1.2E-11	1.6E-10	5.1E-12	1.1E-10	6.5E-10	0.
METHANOL	3.1E-11	2.9E-10	1.1E-10	3.2E-10	3.8E-10	2.1E-11	0.
ETHANOL	1.6E-16	3.7E-14	1.2E-13	4.2E-14	3.0E-13	1.8E-13	0.
N2	1.4E-06	1.4E-06	1.6E-06	1.3E-06	1.9E-06	2.2E-06	1.3E-06
NH3	9.6E-08	1.5E-07	1.9E-08	6.1E-07	1.6E-07	4.8E-09	6.0E-30
HCN	5.5E-13	1.2E-11	2.1E-10	6.8E-12	8.7E-11	3.1E-09	0.
NO	2.6E-24	8.1E-25	1.5E-25	3.0E-25	2.1E-25	1.2E-26	6.5E-10
NO2	6.9E-39	0.	0.	0.	0.	0.	4.5E-10
N2O	1.6E-31	5.0E-32	1.0E-32	1.7E-32	1.5E-32	9.3E-34	3.7E-17
NITROUS ACID	2.8E-34	3.1E-35	5.3E-37	7.3E-36	1.6E-36	0.	7.4E-13
NITRIC ACID	0.	0.	0.	0.	0.	0.	9.9E-14
C2N2	2.2E-29	7.3E-27	9.2E-24	9.5E-28	4.4E-25	6.0E-21	0.
HNCO	5.9E-13	3.8E-12	1.2E-11	8.8E-13	6.2E-12	1.2E-11	7.7E-35
FORMAMIDE	1.4E-20	1.1E-19	9.2E-20	7.1E-20	1.8E-19	3.4E-20	0.
GLYCINE	2.5E-25	1.5E-23	1.9E-23	3.9E-24	3.2E-23	3.7E-24	0.
ALANINE	9.0E-32	1.3E-28	1.4E-27	3.4E-29	1.8E-27	2.1E-27	0.
SERINE	9.6E-39	4.2E-36	7.9E-36	4.4E-37	1.2E-35	8.2E-37	0.
ASPARTIC ACID	0.	6.0E-37	7.0E-36	9.6E-39	2.6E-36	1.1E-36	0.
VALINE	0.	1.3E-38	9.4E-36	0.	6.8E-36	8.8E-34	0.
LEUCINE	0.	0.	0.	0.	0.	6.9E-37	0.
FORMYLGLYCINE	1.4E-37	4.6E-35	3.5E-34	1.8E-36	1.5E-34	1.0E-34	0.
OXAMIC ACID	4.3E-28	6.0E-27	5.4E-27	2.3E-28	3.0E-27	2.0E-28	0.
P2	1.0E-33	3.6E-32	6.2E-30	6.0E-31	4.0E-30	2.3E-26	0.
P406	7.3E-07	7.6E-07	8.0E-07	7.9E-07	1.0E-06	1.1E-06	3.2E-36
P4010	3.1E-35	2.8E-37	0.	7.1E-39	0.	0.	6.3E-07
PO	4.4E-24	8.0E-24	1.9E-23	1.3E-23	1.8E-23	7.9E-23	1.2E-38
PO2	4.7E-21	2.6E-21	1.1E-21	1.7E-21	1.3E-21	3.2E-22	3.5E-21
PH3	1.5E-19	1.4E-18	2.3E-18	2.5E-17	1.3E-17	3.0E-17	0.
PCL3	8.5E-36	3.9E-35	4.7E-33	4.0E-35	1.0E-33	3.4E-30	0.
POCL3	2.1E-34	3.0E-34	6.6E-33	1.2E-34	1.7E-33	3.2E-31	6.0E-27
PSCL3	8.2E-37	3.0E-36	1.5E-33	1.2E-36	1.1E-34	2.5E-30	0.
CL2	1.4E-25	1.2E-25	5.2E-25	4.7E-26	2.2E-25	2.7E-24	6.5E-11
HCl	2.9E-06	3.0E-06	3.2E-06	3.1E-06	4.0E-06	4.4E-06	2.5E-06
HgCl	5.5E-24	1.7E-24	3.3E-25	7.1E-25	5.1E-25	3.1E-26	1.2E-09
Cl20	0.	0.	0.	0.	0.	0.	3.5E-20
CH3CL	3.2E-14	8.0E-13	7.1E-12	8.6E-13	6.7E-12	7.6E-11	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
COCL2	1.8E-27	8.3E-27	2.3E-25	5.1E-28	2.3E-26	1.7E-24	2.9E-27
S2	1.1E-17	7.0E-18	1.2E-16	1.1E-18	1.4E-17	6.3E-16	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	2.9E-06	3.0E-06	3.2E-06	3.2E-06	4.0E-06	2.6E-06	0.
SO2	1.8E-15	1.3E-16	1.8E-17	7.9E-18	8.9E-18	1.9E-19	2.9E-08
SO3	5.9E-28	1.3E-29	3.4E-31	3.2E-31	2.0E-31	2.4E-34	2.5E-06
COS	4.7E-09	2.1E-08	5.3E-07	1.2E-09	4.2E-08	1.8E-06	0.
CS2	1.8E-17	2.1E-16	1.2E-13	1.2E-17	2.7E-15	1.4E-11	0.
SULFURCUS ACID	7.9E-33	2.3E-34	1.5E-36	1.5E-35	3.3E-36	0.	5.5E-26
SULFURIC ACID	6.2E-36	5.6E-38	0.	0.	0.	0.	1.1E-14
METHANETHIOL	1.8E-13	4.6E-12	4.1E-11	4.9E-12	3.8E-11	2.6E-10	0.
DIMETHYLSULFIDE	1.4E-20	8.0E-18	6.0E-16	8.9E-18	4.2E-16	3.0E-14	0.
ETHANETHIOL	2.1E-19	1.2E-16	9.1E-15	1.3E-16	6.4E-15	4.5E-13	0.
DIETHYLSULFIDE	1.5E-32	5.0E-27	2.7E-23	5.9E-27	1.0E-23	8.0E-20	0.
OCTANETHIOL	0.	0.	0.	0.	0.	3.8E-32	0.
THIOFORMIC ACID	8.7E-23	5.0E-22	3.2E-21	7.9E-23	9.7E-22	3.8E-21	0.
THIODACETIC ACID	6.2E-28	8.4E-26	4.6E-24	1.4E-26	1.0E-24	4.3E-23	0.
CYCLOPROP.THIOL	5.3E-25	5.5E-21	1.4E-17	2.4E-21	2.0E-18	1.5E-14	0.
CYCLOBUTA.THIOL	6.0E-32	1.5E-26	3.2E-22	6.7E-27	3.4E-23	2.7E-18	0.
CYCLOCAPT.THIOL	5.8E-37	3.4E-30	6.2E-25	1.6E-30	4.8E-26	4.1E-20	0.
CYCLOHEXA.THIOL	0.	3.7E-32	5.6E-26	1.7E-32	3.3E-27	2.9E-20	0.
M.SULFONIC ACID	2.5E-35	1.7E-35	9.3E-37	1.2E-36	1.5E-36	0.	0.
E.SULFINIC ACID	9.5E-20	1.7E-17	2.3E-16	7.4E-18	2.0E-16	7.7E-16	0.
THIOPHEN	3.4E-26	4.9E-21	1.7E-15	3.1E-22	1.2E-17	1.1E-10	0.
BENZENETHIOL	5.8E-34	3.5E-26	3.5E-18	8.7E-28	3.7E-21	3.9E-11	0.
THIOLYCOL	1.7E-31	3.0E-29	4.1E-28	1.3E-29	3.5E-28	1.4E-27	0.
CYSTEINE	0.	8.8E-39	3.9E-37	0.	1.7E-37	1.3E-36	0.
METHIONINE	0.	0.	0.	0.	0.	0.	0.

TABLE 36a

700°K AND 20 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F_i}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-71.087	-19.127	1.466	-5.395	-110.934	-7.872	-73.544
2	2.0	9.0	89.0	-70.964	-18.335	1.423	-5.376	-110.817	-8.627	-73.378
3	2.0	19.0	79.0	-70.758	-17.896	1.347	-5.349	-110.614	-9.011	-73.097
4	2.0	29.0	69.0	-70.498	-17.305	1.246	-5.319	-110.347	-9.244	-72.736
5	2.0	39.0	59.0	-70.145	-17.353	1.101	-5.288	-109.969	-9.434	-72.238
6	2.0	49.0	49.0	-69.596	-17.085	0.859	-5.255	-109.348	-9.636	-71.447
7	2.0	59.0	39.0	-68.280	-16.646	0.237	-5.220	-107.774	-10.003	-69.509
8	2.0	69.0	29.0	-2.951	0.205	-33.461	-5.911	-38.962	-26.813	-19.769
9	2.0	79.0	19.0	-6.479	1.087	-35.760	-8.413	-35.545	-27.823	-21.663
10	2.0	89.0	9.0	-7.647	1.348	-37.154	-9.321	-33.486	-28.209	-22.311
11	2.0	96.0	2.0	-8.143	1.452	-38.946	-9.713	-30.818	-28.393	-22.600
12	10.0	2.0	88.0	-69.171	-19.028	1.356	-5.351	-110.637	-7.884	-73.128
13	10.0	10.0	80.0	-68.974	-18.163	1.280	-5.328	-110.436	-8.704	-72.855
14	10.0	20.0	70.0	-68.655	-17.722	1.151	-5.298	-110.099	-9.084	-72.407
15	10.0	30.0	60.0	-68.185	-17.385	0.949	-5.265	-109.576	-9.357	-71.735
16	10.0	40.0	50.0	-67.269	-16.995	0.525	-5.230	-108.499	-9.675	-70.395
17	10.0	50.0	40.0	-1.157	-0.372	-32.598	-5.333	-40.316	-26.231	-18.612
18	10.0	60.0	30.0	-0.539	-0.133	-33.093	-5.428	-39.494	-26.399	-19.017
19	10.0	70.0	20.0	-0.684	0.066	-33.565	-5.579	-38.767	-26.519	-19.338
20	10.0	80.0	10.0	-4.091	0.949	-35.902	-7.773	-35.277	-27.461	-21.163
21	10.0	88.0	2.0	-5.542	1.280	-36.299	-8.893	-31.712	-27.918	-21.951
22	20.0	2.0	78.0	-67.884	-18.850	1.119	-5.291	-110.014	-7.944	-72.297
23	20.0	10.0	70.0	-67.492	-17.933	0.949	-5.265	-109.576	-8.807	-71.735
24	20.0	20.0	60.0	-66.576	-17.342	0.525	-5.230	-108.499	-9.329	-70.395
25	20.0	30.0	50.0	-0.163	-0.605	-32.677	-5.263	-40.136	-25.996	-18.143
26	20.0	40.0	40.0	0.690	-0.433	-33.178	-5.266	-39.365	-26.090	-18.410
27	20.0	50.0	30.0	1.132	-0.378	-33.500	-5.236	-38.862	-26.059	-18.433
28	20.0	60.0	20.0	1.533	-0.363	-33.854	-5.188	-38.306	-25.979	-18.368
29	20.0	70.0	10.0	2.052	-0.399	-34.404	-5.117	-37.455	-25.836	-18.194
30	22.0	76.0	2.0	6.709	-1.495	-37.456	-5.766	-33.250	-26.228	-17.712
31	18.0	80.0	2.0	-0.644	0.311	-35.939	-5.781	-35.144	-26.512	-19.576
32	30.0	2.0	68.0	-65.814	-18.400	0.354	-5.223	-108.068	-8.256	-69.867
33	30.0	10.0	60.0	1.637	-1.049	-33.369	-5.210	-39.098	-25.549	-17.251
34	30.0	20.0	50.0	4.227	-1.320	-34.703	-5.158	-37.072	-25.204	-16.847
35	30.0	30.0	40.0	6.881	-1.864	-36.139	-5.129	-34.910	-24.598	-16.700
36	30.0	40.0	30.0	6.896	-1.778	-36.238	-5.074	-34.734	-24.573	-16.587
37	30.0	50.0	20.0	6.880	-1.692	-36.375	-5.011	-34.497	-24.532	-16.434
38	30.0	60.0	10.0	6.857	-1.609	-36.649	-4.938	-34.048	-24.468	-16.216
39	30.0	68.0	2.0	6.836	-1.539	-37.433	-4.867	-32.837	-24.397	-15.889
40	40.0	10.0	50.0	7.351	-7.529	-36.258	-5.120	-34.728	-23.918	-16.680
41	40.0	20.0	40.0	7.152	-2.134	-36.207	-5.059	-34.774	-24.190	-16.593
42	40.0	30.0	30.0	7.061	-1.942	-36.240	-4.992	-34.690	-24.248	-16.442
43	40.0	40.0	20.0	6.998	-1.800	-36.339	-4.917	-34.504	-24.237	-16.257
44	40.0	50.0	10.0	6.945	-1.677	-36.579	-4.827	-34.098	-24.180	-16.004
45	40.0	58.0	2.0	6.905	-1.581	-37.329	-4.738	-32.930	-24.099	-15.618

TABLE 36b

700°K AND 20 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	3.2E-02	1.6E-01	2.5E-01	3.3E-01	7.1E-01	6.8E-01	0.
H2	2.4E-02	2.1E-02	1.2E-03	3.5E-01	2.2E-02	2.0E-03	2.0E-17
O2	2.6E-30	7.6E-31	2.0E-33	3.3E-33	6.5E-32	7.3E-34	5.0E-01
WATER	6.7E-01	3.2E-01	9.5E-04	3.3E-01	1.0E-01	9.5E-04	2.5E-01
CO	1.1E-03	3.6E-03	9.2E-02	2.0E-06	4.2E-03	5.4E-02	2.3E-18
CO2	2.7E-01	5.0E-01	6.5E-01	1.8E-05	1.7E-01	2.3E-01	2.5E-01
BENZENE	4.5E-21	2.1E-16	5.2E-04	2.8E-25	8.8E-13	2.1E-03	0.
NAPHTHALENE	1.1E-33	6.9E-26	5.7E-04	0.	7.4E-20	3.4E-03	0.
ASPHALT	0.	0.	1.9E-03	0.	0.	2.4E-02	0.
ACETYLENE	3.0E-17	1.1E-15	1.4E-11	1.2E-18	1.7E-14	2.3E-11	0.
ETHYLENE	9.2E-11	2.9E-09	2.3E-06	5.1E-11	5.0E-08	6.0E-06	0.
ETHANE	2.1E-07	5.8E-06	2.6E-04	1.6E-06	1.1E-04	1.1E-03	0.
FORMIC ACID	5.9E-08	9.5E-08	7.1E-09	5.5E-11	3.4E-08	4.2E-09	4.6E-23
ACETIC ACID	4.8E-09	4.4E-08	9.2E-08	3.4E-12	6.6E-08	8.8E-08	0.
FORMALDEHYDE	1.2E-09	3.8E-19	5.4E-09	3.3E-11	4.6E-09	5.3E-09	0.
ACETALDEHYDE	1.1E-11	1.9E-10	7.8E-09	2.2E-13	9.9E-10	1.2E-08	0.
METHANOL	1.8E-09	4.9E-09	4.0E-10	6.0E-10	6.4E-09	6.6E-10	0.
ETHANOL	5.0E-13	7.6E-12	1.7E-11	1.4E-13	4.1E-11	4.6E-11	0.
N2	1.2E-06	1.3E-06	1.8E-06	8.4E-09	1.8E-06	2.6E-06	1.3E-06
NH3	7.3E-07	6.5E-07	1.0E-08	3.4E-06	8.4E-07	2.7E-08	1.9E-29
HCN	6.0E-13	3.8E-12	5.1E-10	1.0E-14	1.8E-11	7.8E-10	0.
NO	1.4E-24	8.2E-25	4.9E-26	4.4E-27	2.8E-25	3.6E-26	6.5E-10
NO2	2.3E-38	7.0E-39	0.	0.	0.	0.	4.4E-09
N2O	8.0E-31	4.9E-31	3.3E-32	2.1E-34	1.9E-31	2.9E-32	3.7E-16
NITROUS ACID	4.1E-33	1.2E-33	8.7E-37	1.6E-36	1.2E-34	4.9E-37	2.3E-11
NITRIC ACID	0.	0.	0.	0.	0.	0.	3.1E-11
C2N2	1.3E-28	6.2E-27	1.9E-21	2.9E-33	1.3E-25	2.7E-21	0.
HNC2	3.8E-12	1.3E-11	9.1E-11	2.3E-15	1.8E-11	8.3E-11	2.4E-34
FORMAMIDE	1.7E-18	5.1E-18	2.0E-18	1.4E-20	7.5E-18	3.1E-18	0.
GLYCINE	9.6E-21	8.8E-20	5.1E-20	2.2E-24	1.6E-19	7.5E-20	0.
ALANINE	1.8E-25	9.3E-24	1.5E-22	3.1E-29	7.0E-23	3.6E-22	0.
SERINE	1.1E-31	3.2E-30	2.6E-30	6.8E-37	7.0E-30	3.8E-30	0.
ASPARTIC ACID	4.9E-32	4.6E-30	9.6E-29	0.	1.2E-29	8.2E-29	0.
VALINE	8.4E-35	1.4E-31	1.7E-27	8.0E-39	1.8E-29	1.1E-26	0.
LEUCINE	0.	2.0E-35	7.0E-30	0.	1.1E-32	7.3E-29	0.
FORMYLGLYCINE	8.7E-32	2.7E-30	4.0E-29	3.7E-38	5.6E-30	3.5E-29	0.
OXAMIC ACID	5.2E-24	2.9E-23	1.5E-23	3.0E-30	1.4E-23	8.0E-24	0.
P2	4.8E-37	3.2E-30	2.4E-32	1.1E-32	1.5E-34	1.3E-31	0.
P4C'	7.7E-07	8.3E-07	8.8E-07	8.4E-07	1.1E-06	1.3E-06	0.
P4C-	4.3E-32	3.9E-33	2.9E-38	7.3E-38	8.8E-35	0.	6.3E-07
PO	5.7E-26	8.0E-26	3.0E-25	3.1E-25	1.6E-25	5.1E-25	0.
PO2	3.7E-22	2.8E-22	6.4E-23	7.1E-23	1.6E-22	5.5E-23	3.5E-23
PH3	2.8E-20	6.1E-20	7.1E-20	2.3E-16	4.5E-19	3.6E-19	0.
PCl3	2.6E-34	1.0E-33	7.9E-30	1.0E-33	1.5E-32	2.8E-29	0.
POCl3	4.0E-32	8.4E-32	3.3E-29	5.4E-33	3.6E-31	6.9E-29	1.9E-25
PSCl3	1.4E-34	6.8E-34	2.9E-29	4.3E-35	1.2E-32	1.6E-28	0.
Cl2	8.2E-25	1.1E-24	2.2E-23	7.0E-26	1.8E-24	2.8E-23	6.4E-10
HCl	3.1E-06	3.3E-06	3.5E-06	3.4E-06	4.4E-06	5.2E-06	2.5E-06
HClL	3.5E-23	2.0E-23	1.1E-24	1.5E-24	7.9E-24	9.8E-25	1.2E-08
Cl2O	0.	0.	0.	0.	0.	0.	3.5E-18
CH3Cl	1.8E-12	1.1E-11	3.2E-10	1.5E-12	6.0E-11	7.7E-10	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
COCl2	1.8E-25	7.9E-25	4.0E-22	2.8E-29	1.5E-24	3.0E-22	2.9E-25
S2	3.4E-18	5.1E-18	1.6E-16	2.1E-20	7.9E-18	4.1E-16	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	3.1E-06	3.3E-06	1.1E-06	3.4E-06	4.4E-06	2.8E-06	0.
S02	3.5E-15	1.3E-15	1.9E-17	3.4E-19	1.3E-16	1.1E-17	2.9E-09
S03	7.1E-27	1.3E-27	1.0E-30	2.4E-32	4.2E-29	3.6E-31	2.5E-06
COS	4.2E-09	1.8E-08	2.5E-06	6.2E-13	2.5E-08	2.4E-06	0.
CS2	1.5E-17	1.4E-16	2.1E-12	4.9E-21	8.6E-16	5.5E-12	0.
SULFURCUS ACID	1.8E-30	3.0E-31	1.3E-35	8.7E-35	1.0E-32	7.8E-36	5.5E-25
SULFURIC ACID	6.5E-33	7.7E-34	0.	1.4E-38	7.6E-36	0.	1.1E-12
METHANETHIOL	1.0E-11	6.2E-11	5.4E-10	8.3E-12	3.4E-10	2.4E-09	0.
DIMETHYLSULFIDE	3.9E-17	1.3E-15	3.3E-13	2.4E-17	3.1E-14	2.3E-12	0.
ETHANETHIOL	3.9E-16	2.0E-14	4.9E-12	3.0E-16	4.6E-13	3.5E-11	0.
DIETHYLSULFIDE	1.2E-25	1.3E-22	2.4E-17	3.9E-26	5.0E-20	4.5E-16	0.
OCTANEETHIOL	0.	7.2E-38	8.3E-27	0.	8.7E-33	1.1E-24	0.
THIOFORMIC ACID	1.5E-21	5.5E-21	4.4E-20	3.1E-24	8.4E-21	7.0E-20	0.
THIOACETIC ACID	5.5E-25	1.1E-23	2.6E-21	8.5E-28	7.3E-23	6.6E-21	0.
CYCLUPROP.ThIOL	4.1E-21	8.8E-19	1.1E-13	1.3E-22	7.9E-17	7.4E-13	0.
CYCLORUTA.ThIOL	2.4E-26	3.0E-23	9.9E-17	5.9E-28	1.1E-20	1.1E-15	0.
CYCLOCENTH.ThIOL	1.2E-29	8.2E-26	7.7E-18	2.2E-31	1.3E-22	1.4E-16	0.
CYCLOHEXA.ThIOL	2.8E-31	1.1E-26	2.8E-17	3.8E-33	7.1E-23	8.5E-16	0.
M.SULFONIC ACID	2.9E-31	2.8E-31	3.4E-34	1.1E-35	3.9E-32	3.2E-34	0.
E.SULFINIC ACID	1.6E-15	3.0E-14	3.8E-13	3.5E-17	2.0E-13	1.6E-12	0.
THIOPHENE	3.8E-23	5.9E-20	6.0E-11	4.0E-27	1.9E-17	2.5E-10	0.
BENZENETHIOL	8.9E-29	4.9E-24	6.9E-11	4.4E-34	2.6E-20	4.5E-10	0.
THIOLGLYCOL	2.9E-27	5.3E-26	6.7E-25	6.1E-29	3.6E-25	2.9E-24	0.
CYSTEINE	8.5E-35	5.4E-33	4.7E-31	0.	5.0E-32	1.9E-30	0.
METHIONINE	0.	0.	1.1E-36	0.	0.	1.1E-35	0.

TABLE 37a

1000°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-50.753	-15.643	-4.291	-11.170	-58.573	-18.038	-47.817
2	2.0	9.0	89.0	-50.631	-14.851	-4.333	-11.150	-58.456	-18.794	-47.694
3	2.0	19.0	79.0	-50.425	-14.412	-4.409	-11.121	-58.254	-19.177	-47.486
4	2.0	29.0	69.0	-50.165	-14.121	-4.510	-11.090	-57.987	-19.410	-47.224
5	2.0	39.0	59.0	-49.812	-13.869	-4.655	-11.056	-57.608	-19.600	-46.849
6	2.0	49.0	49.0	-49.263	-13.602	-4.897	-11.020	-56.988	-19.802	-46.301
7	2.0	59.0	39.0	-47.947	-13.162	-5.520	-10.981	-55.414	-20.171	-44.985
8	2.0	69.0	29.0	-14.983	-4.954	-22.149	-11.004	-26.772	-28.442	-16.318
9	2.0	79.0	19.0	-12.787	-4.544	-23.559	-11.068	-24.690	-28.977	-17.268
10	2.0	89.0	9.0	-11.089	-4.361	-24.923	-11.125	-22.672	-29.274	-17.747
11	2.0	96.0	2.0	-1.753	-4.279	-34.117	-11.161	-8.899	-29.432	-17.984
12	10.0	2.0	88.0	-48.838	-15.545	-4.401	-11.124	-58.276	-18.050	-47.509
13	10.0	10.0	80.0	-48.640	-14.679	-4.476	-11.099	-58.075	-18.870	-47.309
14	10.0	20.0	70.0	-48.322	-14.238	-4.605	-11.067	-57.738	-19.251	-46.988
15	10.0	30.0	60.0	-47.852	-13.902	-4.808	-11.032	-57.216	-19.523	-46.499
16	10.0	40.0	50.0	-46.936	-13.511	-5.232	-10.993	-56.139	-19.844	-45.583
17	10.0	50.0	40.0	-14.584	-5.364	-21.469	-10.984	-27.782	-27.991	-15.463
18	10.0	60.0	30.0	-11.600	-4.730	-23.257	-11.050	-25.134	-28.759	-16.865
19	10.0	70.0	20.0	-9.960	-4.502	-24.506	-11.109	-23.290	-29.105	-17.438
20	10.0	80.0	10.0	0.114	-4.370	-34.375	-11.161	-8.512	-29.340	-12.963
21	10.0	88.0	2.0	6.741	-4.294	-42.476	-12.401	-11.094	-29.280	-17.816
22	20.0	2.0	78.0	-47.551	-15.367	-4.638	-11.060	-57.653	-18.109	-46.910
23	20.0	10.0	70.0	-47.159	-14.451	-4.808	-11.032	-57.215	-18.973	-46.499
24	20.0	20.0	60.0	-46.243	-13.658	-5.232	-10.993	-56.139	-19.497	-45.583
25	20.0	30.0	50.0	-13.724	-5.582	-21.558	-10.983	-27.648	-27.772	-15.026
26	20.0	40.0	40.0	-10.784	-4.914	-23.336	-11.049	-25.015	-28.574	-16.494
27	20.0	50.0	30.0	-9.175	-4.663	-24.578	-11.108	-23.181	-28.941	-13.368
28	20.0	60.0	20.0	-9.825	-4.514	-32.742	-11.161	-10.961	-29.198	-17.516
29	20.0	70.0	10.0	6.816	-4.467	-40.912	-12.257	-11.078	-29.140	-15.529
30	22.0	76.0	2.0	6.805	-4.310	-42.320	-13.774	-11.794	-30.664	-19.189
31	18.0	80.0	2.0	6.787	-4.304	-42.381	-12.301	-11.022	-29.131	-17.658
32	30.0	2.0	68.0	-45.480	-14.917	-5.403	-10.985	-55.708	-18.424	-45.225
33	30.0	10.0	60.0	-13.141	-6.092	-21.653	-10.982	-27.506	-27.260	-14.004
34	30.0	20.0	50.0	-10.257	-5.242	-23.416	-11.048	-24.896	-28.246	-15.836
35	30.0	30.0	40.0	-8.683	-4.911	-24.648	-11.108	-23.077	-28.695	-16.673
36	30.0	40.0	30.0	1.445	-4.717	-34.607	-11.160	-11.161	-28.394	-14.061
37	30.0	50.0	20.0	6.918	-4.592	-40.325	-12.178	-11.079	-28.355	-17.198
38	30.0	60.0	10.0	6.882	-4.451	-40.792	-12.188	-10.986	-28.939	-17.291
39	30.0	68.0	2.0	6.838	-4.326	-42.174	-12.067	-10.896	-28.847	-17.357
40	40.0	10.0	50.0	-8.313	-5.455	-24.715	-11.108	-22.976	-28.149	-14.091
41	40.0	20.0	40.0	2.313	-5.063	-35.187	-11.160	-11.162	-28.648	-14.350
42	40.0	30.0	30.0	7.080	-4.888	-40.084	-12.168	-11.082	-28.662	-14.062
43	40.0	40.0	20.0	7.024	-4.711	-40.245	-12.095	-10.988	-28.651	-16.890
44	40.0	50.0	10.0	6.952	-4.525	-40.634	-11.861	-10.870	-28.695	-16.914
45	40.0	58.0	2.0	6.883	-4.359	-41.938	-11.842	-10.754	-28.536	-17.010

TABLE 37b

1000°K AND  $0.2 \times 10^{-3}$  ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	1.1E-13	3.0E-11	2.4E-10	1.4E-05	9.9E-03	8.9E-03	0.
H2	1.1E-01	2.7E-01	2.7E-01	8.0E-01	7.4E-01	6.8E-01	2.1E-09
O2	1.1E-15	2.7E-17	1.9E-18	6.9E-27	1.5E-32	1.9E-32	5.0E-01
WATER	6.0E-01	2.3E-01	6.2E-02	1.1E-05	1.5E-08	1.5E-08	2.5E-01
CO	3.3E-02	2.3E-01	5.1E-01	2.0E-01	2.4E-01	2.8E-01	1.6E-09
CO2	2.5E-01	2.7E-01	1.6E-01	3.8E-06	6.4E-09	8.7E-09	2.5E-01
BENZENE	0.	0.	0.	9.9E-22	2.3E-04	2.6E-04	0.
NAPHTHALENE	0.	0.	0.	1.5E-33	1.4E-04	2.0E-04	0.
ASPHALT	0.	0.	0.	0.	1.0E-02	2.5E-02	0.
ACETYLENE	3.1E-23	1.5E-19	1.0E-17	1.3E-09	8.2E-04	8.6E-04	0.
ETHYLENE	3.4E-25	4.2E-21	2.8E-19	1.1E-10	6.1E-05	5.9E-05	0.
ETHANE	2.2E-29	6.5E-25	4.4E-23	5.0E-14	2.6E-08	2.3E-08	0.
FORMIC ACID	4.0E-12	1.1E-11	6.3E-12	4.4E-16	6.9E-19	8.6E-19	7.8E-20
ACETIC ACID	4.3E-25	1.3E-22	6.1E-22	8.3E-22	1.0E-21	1.2E-21	0.
FORMALDEHYDE	9.5E-13	1.6E-11	3.6E-11	4.2E-11	4.6E-11	5.0E-11	8.7E-28
ACETALDEHYDE	3.4E-26	6.4E-23	1.2E-21	2.6E-17	2.2E-14	2.4E-14	0.
METHANOL	9.3E-19	3.9E-17	8.7E-17	3.0E-16	3.0E-16	3.1E-16	0.
ETHANOL	1.8E-33	8.2E-30	1.5E-28	1.0E-23	7.7E-21	7.7E-21	0.
N2	1.4E-06	1.3E-06	1.1E-06	1.0E-06	1.1E-07	1.3E-07	1.2E-06
NH3	4.7E-12	1.7E-11	1.6E-11	7.8E-11	2.3E-11	2.2E-11	1.2E-23
HCN	1.7E-15	1.1E-13	8.5E-13	9.1E-09	2.4E-06	2.6E-06	4.8E-34
NO	3.5E-15	5.0E-16	1.3E-16	7.2E-21	3.5E-24	4.2E-24	6.7E-08
NO2	1.8E-25	4.1E-27	2.8E-28	9.4E-37	0.	0.	7.4E-11
N2O	4.6E-24	6.2E-25	1.5E-25	8.0E-30	1.3E-33	1.7E-33	8.2E-17
NITROUS ACID	6.5E-25	2.3E-26	1.6E-27	9.1E-36	0.	0.	3.7E-14
NITRILE ACID	7.4E-36	4.0E-38	0.	0.	0.	0.	8.9E-18
C2H2	3.9E-33	6.2E-30	3.7E-28	1.4E-20	1.1E-15	1.4E-15	0.
HNCO	1.9E-15	1.9E-14	4.0E-14	2.5E-14	9.7E-15	1.2E-14	1.1E-26
FORMAMIDE	1.0E-24	4.0E-23	8.4E-23	1.0E-22	5.6E-23	6.4E-23	0.
GLYCINE	0.	2.3E-38	1.1E-37	2.4E-37	9.2E-38	1.1E-37	0.
ALANINE	0.	0.	0.	0.	0.	0.	0.
SERINE	0.	0.	0.	0.	0.	0.	0.
ASPARTIC ACID	0.	0.	0.	0.	0.	0.	0.
VALINE	0.	0.	0.	0.	0.	0.	0.
LEUCINE	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	0.	0.	0.	0.	0.	0.
OXAMIC ACID	3.3E-37	8.9E-36	1.1E-35	0.	0.	0.	0.
P2	3.7E-21	9.4E-19	4.5E-17	2.1E-04	1.2E-06	1.4E-06	0.
P4O6	7.2E-07	6.3E-07	5.6E-07	5.1E-07	1.6E-28	4.8E-28	5.8E-15
P4O10	4.0E-28	2.0E-31	9.3E-34	0.	0.	0.	6.3E-07
PU	8.0E-13	2.0E-12	3.7E-12	4.6E-10	5.2E-14	6.4E-14	1.6E-18
PO2	9.9E-11	3.8E-11	1.9E-11	1.4E-13	2.3E-20	3.2E-20	4.3E-09
PH3	5.7E-18	3.5E-16	2.4E-15	2.6E-08	1.8E-09	1.7E-09	0.
PCl3	6.6E-34	1.8E-33	8.8E-33	2.7E-27	3.8E-28	8.2E-28	1.6E-35
POCl3	3.4E-33	1.5E-33	1.9E-33	3.5E-32	7.0E-36	1.7E-35	1.7E-27
PSCL3	1.7E-36	1.7E-36	6.7E-36	8.4E-29	9.0E-31	3.4E-31	0.
Cl2	2.4E-21	7.6E-22	6.0E-22	1.0E-22	2.4E-22	3.9E-22	9.5E-14
HCl	2.9E-06	2.5E-06	2.2E-06	2.0E-06	2.4E-06	2.9E-06	2.5E-06
HOCl	2.0E-12	2.7E-19	6.4E-20	3.4E-24	5.8E-27	7.9E-27	3.6E-11
Cl2O	9.9E-38	4.7E-39	0.	0.	0.	0.	8.1E-23
CH3Cl	9.7E-23	9.3E-21	6.8E-20	1.2E-15	1.1E-12	1.3E-12	0.
CCl4	0.	0.	0.	0.	0.	0.	0.
COCl2	6.1E-28	1.3E-27	2.3E-27	2.5E-28	4.4E-28	8.4E-28	1.1E-27
S2	1.9E-10	2.4E-11	1.6E-11	2.6E-08	1.6E-10	4.8E-12	7.7E-38
SB	0.	0.	0.	0.	0.	0.	0.
H2S	2.9E-06	2.5E-06	2.1E-06	2.6E-04	1.8E-05	2.9E-06	1.2E-27
SO2	2.7E-07	2.3E-09	1.4E-10	2.1E-17	3.3E-24	7.2E-25	2.5E-06
S3	2.5E-16	3.3E-19	5.4E-21	4.7E-32	0.	0.	4.8E-08
COS	2.8E-08	6.9E-08	1.3E-07	2.0E-06	1.8E-07	3.8E-08	2.7E-29
CS2	7.0E-16	4.0E-15	2.3E-14	2.5E-07	1.2E-06	3.8E-08	0.
SULFURUS ACID	1.3E-24	4.2E-27	7.0E-29	0.	0.	0.	4.9E-24
SULFURIC ACID	1.1E-26	5.5E-30	2.4E-32	0.	0.	0.	8.7E-19
METHANETHIOL	4.5E-22	4.4E-20	3.0E-19	7.1E-13	3.8E-11	5.9E-12	0.
DIMETHYLSULFIDE	4.6E-38	4.9E-34	2.8E-32	1.3E-21	5.2E-17	7.8E-18	0.
ETHANETHIOL	4.5E-37	4.8E-33	2.7E-31	1.2E-20	5.1E-16	7.6E-17	0.
DIETHYLSULFIDE	0.	0.	0.	3.4E-37	7.9E-27	1.1E-27	0.
OCTANETHIOL	0.	0.	0.	0.	0.	0.	0.
THIOFORMIC ACID	8.4E-23	5.1E-22	9.5E-22	4.5E-20	3.8E-21	7.2E-22	0.
THIACETIC ACID	0.	2.0E-36	3.0E-35	2.8E-29	1.8E-27	3.3E-28	0.
CYCLOPROP.THIOL	0.	0.	8.7E-37	2.6E-22	8.8E-15	1.4E-15	0.
CYCLOBUTA.THIOL	0.	0.	0.	5.1E-31	1.3E-20	2.0E-21	0.
CYCLOCENT.PHIOL	0.	0.	0.	0.	1.2E-26	1.8E-27	0.
CYCLOHEXA.THIOL	0.	0.	0.	0.	1.7E-28	2.5E-29	0.
M.SULFONIC ACID	1.4E-37	5.1E-38	6.8E-39	0.	0.	0.	0.
E.SULFINIC ACID	7.8E-39	1.3E-35	2.0E-34	5.4E-28	3.2E-26	5.4E-27	0.
THIOPHENF	0.	0.	2.4E-37	1.7E-19	4.8E-09	9.0E-10	0.
BENZENETHIOL	0.	0.	0.	1.1E-27	2.0E-11	3.9E-12	0.
THIOLGLYCOL	0.	0.	0.	5.9E-35	3.5E-33	5.9E-34	0.
CYSTEINE	0.	0.	0.	0.	0.	0.	0.
METHIONINE	0.	0.	0.	0.	0.	0.	0.

TABLE 38a

1000°K AND 0.2 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\frac{F}{RT}$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-50.753	-13.916	-0.837	-7.717	-65.481	-12.859	-48.399
2	2.0	9.0	89.0	-50.631	-13.124	-0.880	-7.697	-65.364	-13.614	-48.257
3	2.0	19.0	79.0	-50.425	-12.685	-0.955	-7.667	-65.161	-13.998	-48.018
4	2.0	29.0	69.0	-50.165	-12.394	-1.056	-7.636	-64.894	-14.231	-47.716
5	2.0	39.0	59.0	-49.812	-12.143	-1.202	-7.603	-64.516	-14.421	-47.308
6	2.0	49.0	49.0	-49.263	-11.875	-1.443	-7.566	-63.895	-14.623	-46.677
7	2.0	59.0	39.0	-47.947	-11.435	-2.066	-7.527	-62.321	-14.990	-45.204
8	2.0	69.0	29.0	-8.076	-1.500	-22.149	-7.550	-25.045	-24.988	-16.323
9	2.0	79.0	19.0	-5.879	-1.093	-23.559	-7.624	-22.962	-25.525	-17.270
10	2.0	89.0	9.0	-4.182	-0.967	-24.923	-7.689	-20.945	-25.821	-17.750
11	2.0	96.0	2.0	-0.969	-0.829	-28.172	-7.725	-16.086	-25.959	-17.966
12	10.0	2.0	88.0	-48.838	-13.818	-0.947	-7.670	-65.184	-12.871	-48.044
13	10.0	10.0	80.0	-48.640	-12.952	-1.022	-7.646	-64.983	-13.691	-47.815
14	10.0	20.0	70.0	-48.322	-12.511	-1.151	-7.613	-64.646	-14.072	-47.446
15	10.0	30.0	60.0	-47.852	-12.175	-1.354	-7.578	-64.123	-14.343	-46.904
16	10.0	40.0	50.0	-46.936	-11.784	-1.778	-7.539	-63.047	-14.665	-45.865
17	10.0	50.0	40.0	-7.676	-1.910	-21.469	-7.530	-26.055	-24.535	-15.464
18	10.0	60.0	30.0	-4.692	-1.276	-23.257	-7.602	-23.407	-25.303	-16.868
19	10.0	70.0	20.0	-3.057	-1.048	-24.502	-7.667	-21.568	-25.648	-17.439
20	10.0	80.0	10.0	0.112	-0.326	-27.524	-7.714	-17.054	-25.850	-17.758
21	10.0	88.0	2.0	2.982	-0.957	-31.670	-7.617	-10.774	-25.569	-17.449
22	20.0	2.0	78.0	-47.551	-13.640	-1.184	-7.606	-64.561	-12.930	-47.356
23	20.0	10.0	70.0	-47.159	-12.724	-1.354	-7.578	-64.123	-13.794	-46.904
24	20.0	20.0	60.0	-46.243	-12.131	-1.778	-7.539	-63.047	-14.318	-45.865
25	20.0	30.0	50.0	-6.816	-2.128	-21.558	-7.530	-25.921	-24.316	-15.059
26	20.0	40.0	40.0	-3.876	-1.460	-23.336	-7.599	-23.288	-25.118	-16.523
27	20.0	50.0	30.0	-2.273	-1.269	-24.574	-7.661	-21.460	-25.486	-17.136
28	20.0	60.0	20.0	0.810	-1.077	-27.496	-7.707	-17.097	-25.695	-17.455
29	20.0	70.0	10.0	4.371	-1.228	-31.368	-7.631	-11.207	-25.217	-16.847
30	22.0	76.0	2.0	5.435	-1.331	-33.693	-8.637	-8.037	-26.387	-17.899
31	18.0	80.0	2.0	5.286	-1.296	-33.629	-7.596	-7.748	-24.886	-16.427
32	30.0	2.0	68.0	-45.480	-13.190	-1.949	-7.531	-62.615	-13.243	-45.469
33	30.0	10.0	60.0	-6.233	-2.638	-21.653	-7.528	-25.779	-23.807	-14.140
34	30.0	20.0	50.0	-3.349	-1.788	-23.416	-7.595	-23.169	-24.790	-15.838
35	30.0	30.0	40.0	-1.775	-1.457	-24.648	-7.658	-21.350	-25.240	-16.675
36	30.0	40.0	30.0	1.476	-1.287	-27.741	-7.706	-16.730	-25.492	-17.087
37	30.0	50.0	20.0	5.474	-1.564	-31.814	-7.759	-10.547	-24.919	-16.267
38	30.0	60.0	10.0	5.538	-1.409	-32.301	-7.631	-9.749	-24.743	-16.152
39	30.0	68.0	2.0	5.518	-1.363	-33.606	-7.478	-7.720	-24.564	-16.048
40	40.0	10.0	50.0	-1.405	-2.01	-24.715	-7.654	-21.249	-24.695	-14.093
41	40.0	20.0	40.0	2.370	-1.643	-28.339	-7.710	-15.836	-25.146	-16.464
42	40.0	30.0	30.0	5.692	-1.819	-31.712	-7.803	-10.721	-24.751	-15.932
43	40.0	40.0	20.0	5.677	-1.692	-31.869	-7.686	-10.427	-24.642	-15.899
44	40.0	50.0	10.0	5.634	-1.547	-32.208	-7.520	-9.840	-24.476	-15.823
45	40.0	58.0	2.0	5.584	-1.406	-33.417	-7.329	-7.940	-24.266	-15.696

TABLE 38b

1000°K AND 0.2 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	1.1E-07	3.0E-05	2.4E-04	1.4E-02	2.9E-01	3.5E-01	0.
H2	1.1E-01	2.7E-01	2.7E-01	7.8E-01	4.3E-01	2.6E-01	6.8E-11
O2	1.1E-18	2.7E-20	1.9E-21	6.2E-24	2.8E-27	4.4E-28	5.0E-01
WATER	6.0E-01	2.3E-01	6.2E-02	1.0E-02	1.2E-04	2.9E-05	2.5E-01
CO	3.3E-02	2.3E-01	5.1E-01	1.9E-01	2.9E-01	3.6E-01	4.9E-11
CO2	2.5E-01	2.7E-01	1.6E-01	3.4E-03	1.1E-04	5.4E-05	2.5E-01
BENZENE	1.3E-38	1.5E-27	4.6E-22	9.2E-16	1.9E-05	4.9E-03	0.
NAPHTHALENE	0.	0.	1.2E-34	1.4E-24	3.8E-07	6.5E-03	0.
ASPHALT	0.	0.	0.	0.	1.6E-12	1.3E-02	0.
ACETYLENE	3.1E-17	1.5E-13	1.0E-11	1.3E-09	3.6E-06	2.3E-05	0.
ETHYLENE	3.4E-16	4.2E-12	2.8E-10	1.0E-07	1.5E-04	6.0E-04	0.
ETHANE	2.2E-17	6.5E-13	4.4E-11	4.7E-08	3.8E-05	9.3E-05	0.
FORMIC ACID	4.0E-09	1.1E-08	6.3E-09	3.8E-10	6.8E-12	2.1E-12	2.5E-18
ACETIC ACID	4.3E-16	1.3E-13	6.1E-13	7.1E-13	4.9E-13	3.0E-13	0.
FORMALDEHYDE	9.5E-10	1.6E-08	3.6E-08	3.8E-08	3.2E-08	2.5E-08	8.7E-28
ACETALDEHYDE	3.4E-17	6.4E-14	1.2E-12	2.4E-11	7.7E-10	1.2E-09	0.
METHANOL	9.3E-13	3.9E-11	8.7E-11	2.7E-10	1.2E-10	5.9E-11	0.
ETHANOL	1.8E-21	8.2E-18	1.5E-16	8.9E-15	1.6E-13	1.5E-13	0.
N2	1.4E-06	1.3E-06	1.1E-06	1.0E-06	1.2E-06	1.2E-06	1.2E-06
NH3	4.7E-09	1.7E-08	1.6E-08	7.0E-08	3.3E-08	1.6E-08	6.7E-23
HCN	1.7E-12	1.1E-10	8.4E-10	8.9E-09	5.1E-07	1.3E-06	8.5E-35
NO	1.1E-16	1.6E-17	4.0E-18	2.1E-19	5.0E-21	2.0E-21	6.7E-08
NO2	5.7E-27	1.3E-28	8.8E-30	2.6E-32	1.3E-35	2.0E-36	2.3E-09
N2O	4.6E-24	6.2E-25	1.5E-25	7.4E-27	1.9E-28	7.4E-29	2.6E-15
NITROUS ACID	6.5E-25	2.3E-26	1.6E-27	8.0E-30	2.9E-33	3.6E-34	6.7E-12
NITRIC ACID	7.4E-36	4.0E-38	0.	0.	0.	0.	5.0E-14
C2N2	3.5E-27	6.1E-24	3.6E-22	1.4E-20	8.4E-17	8.6E-16	0.
HNCO	1.9E-12	1.9E-11	3.9E-11	2.4E-11	2.9E-11	2.8E-11	6.4E-26
FORMAMIDE	1.6E-18	4.0E-17	8.4E-17	1.5E-16	9.7E-17	5.9E-17	0.
GLYCINE	5.5E-29	2.3E-26	1.1E-25	2.0E-25	1.1E-25	5.3E-26	0.
ALANINE	1.7E-38	7.9E-34	3.0E-32	1.1E-30	2.3E-29	2.1E-29	0.
SERINE	0.	0.	2.3E-38	4.7E-38	2.1E-38	8.0E-39	0.
ASPARTIC ACID	0.	0.	0.	0.	0.	0.	0.
VALINE	0.	0.	0.	0.	1.5E-36	5.5E-36	0.
LEUCINE	0.	0.	0.	0.	0.	0.	0.
FORMYLGLYCINE	0.	5.8E-36	5.9E-35	4.1E-35	3.4E-35	2.0E-35	0.
OXAMIC ACID	3.3E-28	8.9E-27	1.1E-26	4.6E-28	8.6E-30	2.6E-30	0.
P2	1.2E-22	3.0E-20	1.4E-18	7.7E-15	9.2E-10	1.7E-08	0.
P4C6	7.2E-07	6.3E-07	5.6E-07	5.2E-07	7.2E-07	9.1E-07	5.8E-21
P4O10	4.0E-28	2.0E-31	9.3E-34	8.7E-39	0.	0.	6.3E-07
PO	4.5E-15	1.1E-14	2.1E-14	8.5E-14	6.3E-13	1.1E-12	5.2E-23
PO2	5.6E-13	2.1E-13	1.1E-13	2.5E-14	4.0E-15	2.6E-15	4.3E-12
PH3	1.0E-15	6.2E-14	4.4E-13	1.6E-10	2.2E-08	4.6E-08	0.
PCL3	1.2E-31	3.3E-31	1.6E-30	1.8E-29	4.3E-26	7.6E-25	8.8E-35
POCL3	6.1E-31	2.6E-31	3.4E-31	2.3E-31	1.1E-29	7.8E-29	3.0E-25
PSCL3	3.0E-34	2.9E-34	1.7E-33	4.6E-33	2.7E-29	9.8E-28	0.
CL2	2.4E-21	7.6E-22	6.0E-22	1.8E-22	6.3E-22	1.6E-21	3.0E-12
HCL	2.9E-06	2.5E-06	2.2E-06	2.1E-06	2.9E-06	3.7E-06	2.5E-06
HOCL	2.0E-18	2.7E-19	6.4E-20	3.3E-21	9.9E-23	4.9E-23	1.1E-09
CL2O	9.9E-38	4.8E-39	0.	0.	0.	0.	8.1E-20
CH3CL	9.7E-17	9.4E-15	6.8E-14	1.2E-12	6.5E-11	1.6E-10	0.
CCL4	0.	0.	0.	0.	0.	0.	0.
COCL2	6.2E-25	1.3E-24	2.3E-24	2.5E-25	1.4E-24	4.4E-24	1.1E-24
S2	1.8E-13	2.2E-14	1.6E-14	1.9E-15	1.2E-14	4.7E-14	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	2.9E-06	2.5E-06	2.1E-06	2.1E-06	2.8E-06	3.5E-06	2.3E-29
SO2	2.7E-10	2.3E-12	1.4E-13	1.5E-16	1.7E-19	5.4E-20	1.6E-06
SO3	2.5E-19	3.2E-22	5.4E-24	3.3E-28	8.0E-33	9.7E-34	9.6E-07
COS	2.8E-08	6.7E-08	1.3E-07	1.6E-08	6.0E-08	1.5E-07	5.3E-31
CS2	7.0E-16	3.7E-15	2.3E-14	1.7E-14	7.5E-12	9.6E-11	0.
SULFURIC ACID	1.3E-24	4.1E-27	7.0E-29	1.2E-32	1.6E-37	1.2E-38	3.1E-21
SULFURIC ACID	1.1E-26	5.4E-30	2.4E-32	2.4E-37	0.	0.	1.7E-14
METHANETHIOL	4.5E-16	4.3E-14	3.0E-13	5.7E-12	3.0E-10	7.3E-10	0.
DIMETHYLSULFIDE	4.6E-26	4.8E-22	2.8E-20	9.9E-18	2.0E-14	9.8E-14	0.
ETHANETHIOL	4.5E-25	4.6E-21	2.7E-19	9.6E-17	2.0E-13	9.5E-13	0.
DIETHYLSULFIDE	0.	4.9E-36	1.9E-32	2.5E-27	7.6E-21	1.5E-19	0.
OCTANETHIOL	0.	0.	0.	0.	2.3E-34	6.8E-32	0.
THIOFORMIC ACID	8.4E-20	5.0E-19	9.4E-19	3.4E-19	7.1E-19	1.1E-18	0.
THIOACETIC ACID	3.0E-30	1.9E-27	3.0E-26	2.1E-25	1.7E-23	5.2E-23	0.
CYCLUPROP. THIOL	3.9E-30	1.8E-24	8.7E-22	2.0E-18	2.9E-13	4.6E-12	0.
CYCLOBUTA. THIOL	0.	2.2E-32	8.5E-29	3.0E-24	2.1E-17	6.6E-16	0.
CYCLOPENT. THIOL	0.	0.	5.3E-36	4.6E-30	9.9E-22	6.1E-20	0.
CYCLOHEXA. THIOL	0.	0.	5.2E-39	8.6E-32	7.1E-22	8.7E-20	0.
M. SULFONIC ACID	1.4E-31	4.9E-32	6.8E-33	2.3E-35	1.2E-38	0.	0.
E. SULFINIC ACID	7.8E-27	1.2E-23	2.0E-22	3.9E-21	1.7E-19	3.3E-19	0.
THIOPHENNE	7.4E-33	6.2E-26	2.4E-22	1.3E-18	2.4E-11	2.0E-09	0.
DENZENETHIOL	0.	4.8E-35	1.2E-29	8.5E-24	4.3E-13	2.2E-10	0.
THIUGLYCOL	8.6E-34	1.4E-30	2.2E-29	4.3E-28	1.9E-26	3.6E-26	0.
CYSTEINE	0.	0.	0.	0.	2.2E-38	4.2E-38	0.
METHIONINE	0.	0.	0.	0.	0.	0.	0.

TABLE 39a

1000°K AND 20 ATM. PRESSURE - PARTIAL MOLAL FREE ENERGIES OF THE ELEMENTS,  $\bar{F}_i/RT$ , FOR 45 SYSTEMS OF C, H, O, N, P, S, AND Cl. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

NO.	MOLE PERCENTAGE			FREE ENERGIES (F/MOLE)						
	C	H	O	C	H	O	N	P	Cl	S
1	2.0	2.0	96.0	-50.753	-12.765	1.466	-5.423	-70.086	-9.405	-49.916
2	2.0	9.0	89.0	-50.631	-11.973	1.423	-5.402	-69.969	-10.160	-49.868
3	2.0	19.0	79.0	-50.425	-11.534	1.347	-5.371	-69.767	-10.544	-49.595
4	2.0	29.0	69.0	-50.165	-11.243	1.246	-5.339	-69.500	-10.777	-49.247
5	2.0	39.0	59.0	-49.812	-10.991	1.101	-5.304	-69.121	-10.967	-48.769
6	2.0	49.0	49.0	-49.263	-10.723	0.859	-5.266	-68.500	-11.169	-48.017
7	2.0	59.0	39.0	-47.947	-10.284	0.237	-5.224	-66.926	-11.539	-46.223
8	2.0	69.0	29.0	-3.615	0.783	-22.097	-5.510	-23.970	-22.659	-16.280
9	2.0	79.0	19.0	-2.682	1.142	-23.247	-6.032	-22.263	-23.090	-17.074
10	2.0	89.0	9.0	-3.192	1.351	-24.452	-6.497	-20.478	-23.390	-17.582
11	2.0	96.0	2.0	-3.633	1.452	-26.227	-6.878	-17.836	-23.567	-17.862
12	10.0	2.0	88.0	-48.838	-12.667	1.356	-5.375	-69.789	-9.417	-49.625
13	10.0	12.0	80.0	-48.640	-11.801	1.280	-5.349	-69.588	-10.236	-49.361
14	10.0	20.0	70.0	-48.322	-11.360	1.151	-5.315	-69.251	-10.617	-48.931
15	10.0	30.0	60.0	-47.852	-11.023	0.949	-5.278	-68.728	-10.889	-48.289
16	10.0	40.0	50.0	-46.936	-10.633	0.525	-5.238	-67.652	-11.211	-47.034
17	10.0	50.0	40.0	-3.128	0.379	-21.440	-5.306	-24.946	-22.217	-15.438
18	10.0	60.0	30.0	-1.095	0.457	-22.702	-5.578	-23.062	-22.736	-16.433
19	10.0	70.0	20.0	-0.650	1.001	-23.250	-5.721	-22.233	-22.844	-16.687
20	10.0	80.0	10.0	-0.615	1.130	-23.943	-5.888	-21.182	-22.928	-16.899
21	10.0	88.0	2.0	-1.073	1.286	-25.675	-6.225	-18.590	-23.105	-17.232
22	20.0	2.0	78.0	-47.551	-12.488	1.119	-5.307	-69.166	-9.476	-48.825
23	20.0	10.0	70.0	-47.159	-11.573	0.949	-5.278	-68.728	-10.340	-48.289
24	20.0	20.0	60.0	-46.243	-10.980	0.525	-5.237	-67.652	-10.864	-47.034
25	20.0	30.0	50.0	-2.264	0.161	-21.530	-5.267	-24.812	-21.998	-15.001
26	20.0	40.0	40.0	-0.179	0.637	-22.772	-5.417	-22.958	-22.511	-16.016
27	20.0	50.0	30.0	0.462	0.741	-23.264	-5.450	-22.207	-22.568	-16.175
28	20.0	60.0	20.0	0.953	0.777	-23.740	-5.426	-21.473	-22.523	-16.163
29	20.0	70.0	10.0	1.569	0.754	-24.483	-5.334	-20.326	-22.371	-15.986
30	22.0	76.0	2.0	4.734	0.100	-28.264	-5.943	-14.994	-23.070	-16.051
31	18.0	80.0	2.0	1.655	0.815	-25.768	-5.301	-18.368	-22.310	-15.962
32	30.0	2.0	68.0	-45.480	-12.038	0.354	-5.229	-67.220	-9.792	-46.549
33	30.0	10.0	60.0	-1.641	-0.340	-21.646	-5.234	-24.637	-21.498	-14.133
34	30.0	20.0	50.0	0.725	0.310	-23.061	-5.326	-22.531	-22.215	-15.461
35	30.0	30.0	40.0	1.571	0.398	-23.669	-5.335	-21.615	-22.281	-15.620
36	30.0	40.0	30.0	2.418	0.350	-24.350	-5.298	-20.580	-22.178	-15.496
37	30.0	50.0	20.0	4.144	0.400	-25.915	-5.232	-18.211	-21.784	-14.931
38	30.0	60.0	10.0	4.943	-0.064	-27.039	-5.113	-16.461	-21.423	-14.439
39	30.0	68.0	2.0	4.948	0.029	-28.310	-4.961	-14.478	-21.214	-14.141
40	40.0	10.0	50.0	2.821	-0.195	-24.388	-5.337	-20.571	-21.823	-14.941
41	40.0	20.0	40.0	4.094	-0.259	-25.506	-5.343	-18.890	-21.748	-14.917
42	40.0	30.0	30.0	5.101	-0.387	-26.518	-5.297	-17.338	-21.484	-14.645
43	40.0	40.0	20.0	5.107	-0.282	-26.677	-5.178	-17.041	-21.349	-14.446
44	40.0	50.0	10.0	5.076	-0.155	-26.997	-5.017	-16.480	-21.154	-14.168
45	40.0	58.0	2.0	5.035	-0.024	-28.136	-4.830	-14.678	-20.914	-13.816

TABLE 39b

1000°K AND 20 ATM. PRESSURE - EQUILIBRIUM CONCENTRATIONS IN MOLE FRACTIONS OF SELECTED COMPOUNDS CONTAINING C, H, O, N, P, S, AND Cl WITH SEVEN SELECTED RELATIVE ABUNDANCE RATIOS OF C, H, AND O. N, P, S, AND Cl CONSTITUTE 0.0001% OF THE TOTAL NUMBER OF MOLES OF ALL ELEMENTS.

COMPOUND	A	B	C	D	E	F	G
METHANE	9.8E-04	5.3E-02	1.2E-01	2.4E-01	4.8E-01	5.3E-01	0.
H2	1.1E-01	1.8E-01	1.1E-01	4.8E-01	2.3E-01	4.4E-02	6.8E-12
O2	1.2E-20	8.3E-22	1.4E-22	8.0E-23	2.7E-23	1.6E-25	5.0E-01
WATER	6.1E-01	2.7E-01	6.0E-02	2.2E-01	6.1E-02	9.3E-04	2.5E-01
CO	3.2E-02	1.6E-01	3.8E-01	3.3E-02	1.7E-01	3.8E-01	4.9E-12
CO2	2.5E-01	3.4E-01	3.2E-01	2.1E-02	6.3E-02	1.1E-02	2.5E-01
BENZENE	8.4E-23	1.9E-14	1.6E-10	2.1E-14	1.4E-09	6.3E-03	0.
NAPHTHALENE	4.0E-36	2.0E-22	1.2E-15	1.3E-22	2.0E-14	1.3E-02	0.
ASPHALT	0.	0.	8.5E-33	0.	5.8E-31	5.5E-03	0.
ACETYLENE	2.7E-13	1.7E-10	3.4E-09	1.9E-10	6.9E-09	1.1E-06	0.
ETHYLENE	2.9E-10	3.0E-07	3.8E-06	8.9E-07	1.6E-05	5.1E-04	0.
ETHANE	1.8E-09	3.1E-06	2.4E-05	2.5E-05	2.1E-04	1.3E-03	0.
FORMIC ACID	5.9E-07	3.7E-07	5.2E-07	1.5E-07	2.1E-07	7.1E-09	2.5E-17
ACETIC ACID	3.9E-10	2.8E-08	5.9E-08	8.0E-09	4.8E-08	9.3E-09	0.
FORMALDEHYDE	9.0E-08	7.6E-07	1.1E-06	4.1E-07	1.0E-06	4.4E-07	8.7E-28
ACETALDEHYDE	3.0E-11	8.1E-09	4.2E-08	7.5E-09	7.6E-08	1.9E-07	0.
METHANOL	8.6E-09	1.2E-07	1.1E-07	1.8E-07	2.0E-07	1.7E-08	5.3E-39
ETHANOL	1.5E-13	6.9E-11	2.2E-10	1.7E-10	8.2E-10	4.0E-10	0.
N2	1.2E-06	9.9E-07	1.2E-06	3.8E-07	1.2E-06	1.8E-06	1.2E-06
NH3	4.2E-07	8.2E-07	4.3E-07	2.2E-06	1.3E-06	1.4E-07	2.1E-22
HCN	1.4E-10	3.2E-09	1.6E-08	2.1E-09	2.2E-08	3.6E-07	2.7E-35
NO	1.0E-17	2.5E-17	1.1E-18	4.8E-19	4.8E-19	4.7E-20	6.7E-08
NO2	5.6E-28	3.5E-29	6.3E-30	2.1E-30	1.2E-30	9.3E-33	2.3E-08
N2O	4.0E-24	8.5E-25	4.1E-25	1.0E-25	1.8E-25	2.2E-26	2.6E-14
NITROUS ACID	6.3E-25	5.1E-26	7.2E-27	5.0E-27	2.0E-27	6.7E-30	2.1E-10
NITRIC ACID	7.3E-36	1.6E-37	9.0E-39	4.8E-39	0.	0.	1.6E-11
C2N2	2.7E-23	7.9E-21	3.1E-19	1.3E-21	3.1E-19	4.0E-16	0.
HNCO	1.7E-10	9.7E-10	1.7E-09	2.0E-10	1.2E-09	1.5E-09	2.0E-25
FORMAMIDE	1.4E-14	1.4E-13	1.7E-13	7.3E-14	2.2E-13	5.3E-14	0.
GLYCINE	4.5E-21	3.7E-19	6.7E-19	1.1E-19	7.8E-19	8.3E-20	0.
ALANINE	1.3E-26	3.4E-23	2.2E-22	1.7E-23	5.1E-22	3.1E-22	0.
SERINE	2.5E-31	1.7E-28	4.5E-28	2.7E-29	4.7E-28	2.2E-29	0.
ASPARTIC ACID	4.6E-33	1.6E-29	1.0E-28	5.1E-31	4.6E-29	5.0E-30	0.
VALINE	1.6E-37	4.3E-31	3.5E-29	6.5E-31	3.4E-28	6.7E-27	0.
LEUCINE	0.	6.6E-35	1.9E-32	1.8E-34	3.8E-31	4.3E-29	0.
FORMYLGLYCINE	1.6E-29	6.5E-27	2.0E-26	3.9E-28	1.4E-26	3.5E-27	0.
OXAMIC ACID	4.9E-22	3.8E-21	4.5E-21	1.3E-22	1.1E-21	4.8E-23	0.
P2	1.1E-23	5.7E-22	8.4E-21	2.4E-20	1.1E-19	2.5E-16	0.
P4C6	7.2E-07	7.0E-07	6.9E-07	7.5E-07	9.0E-07	1.0E-06	5.8E-25
P4C10	4.5E-28	2.1E-30	5.8E-32	2.1E-32	2.9E-33	1.2E-37	6.3E-07
PU	1.4E-16	2.7E-16	4.2E-16	4.9E-16	6.8E-16	2.5E-15	5.2E-26
PU2	1.8E-14	9.1E-15	5.8E-15	5.2E-15	4.1E-15	1.2E-15	4.3E-14
PH3	3.0E-14	4.7E-13	8.7E-13	1.2E-11	9.2E-12	3.8E-11	0.
PCL3	3.7E-30	1.1E-29	8.6E-29	1.9E-29	2.4E-28	2.0E-25	2.8E-34
PUCL3	2.0E-29	1.6E-29	5.0E-29	8.3E-30	6.1E-29	3.9E-27	9.6E-24
PSCL3	9.8E-33	1.7E-32	1.9E-31	1.2E-32	3.6E-31	1.4E-27	0.
CL2	2.5E-21	1.4E-21	2.2E-21	6.1E-22	1.9E-21	1.2E-20	3.0E-11
HCL	2.9E-06	2.8E-06	2.8E-06	3.0E-06	3.6E-06	4.1E-06	2.5E-06
HGCL	2.0E-18	5.2E-19	2.1E-19	1.7E-19	1.2E-19	1.1E-20	1.1E-08
CL2O	1.1E-37	1.5E-38	1.3E-38	0.	0.	0.	8.1E-18
CH3CL	9.0E-13	2.8E-11	9.8E-11	5.2E-11	2.6E-10	1.7E-09	0.
CCL4	0.	0.	0.	0.	0.	1.3E-38	0.
COCL2	6.2E-23	1.7E-22	6.5E-22	1.5E-23	2.4E-22	3.6E-21	1.1E-22
S2	1.9E-15	6.1E-16	1.4E-15	1.0E-16	6.5E-16	1.4E-14	0.
S8	0.	0.	0.	0.	0.	0.	0.
H2S	2.9E-06	2.7E-06	2.5E-06	3.0E-06	3.5E-06	3.2E-06	5.2E-31
SO2	3.0E-12	1.2E-13	2.9E-14	4.0E-15	3.9E-15	1.1E-16	3.5E-07
S03	2.8E-21	2.9E-23	2.9E-24	3.6E-25	1.8E-25	3.9E-28	2.2E-06
COS	2.8E-08	7.9E-08	2.7E-07	6.5E-09	8.4E-08	8.9E-07	1.2E-32
CS2	6.9E-16	4.2E-15	5.3E-14	4.0E-16	2.5E-14	1.6E-11	0.
SULFURCUS ACID	1.4E-24	2.0E-26	1.5E-27	8.2E-28	1.9E-28	8.1E-32	7.0E-20
SULFURIC ACID	1.2E-26	5.6E-29	1.4E-30	5.6E-31	7.8E-32	2.6E-36	3.9E-12
METHANETHIOL	4.2E-12	1.3E-10	4.1E-10	2.4E-10	1.2E-09	6.2E-09	0.
DIMETHYLSULFIDE	3.9E-18	3.8E-15	4.4E-14	1.2E-14	2.6E-13	7.6E-12	0.
ETHANETHIOL	3.8E-17	3.6E-14	4.3E-13	1.2E-13	2.5E-12	7.4E-11	0.
DIETHYLSULFIDE	2.8E-28	2.8E-22	4.1E-20	2.8E-21	9.9E-19	9.5E-16	0.
OCTAETHIOL	0.	3.2E-37	7.5E-33	7.8E-35	3.1E-30	3.1E-24	0.
THIOFORMIC ACID	8.2E-18	3.9E-17	8.4E-17	8.6E-18	5.2E-17	1.1E-16	0.
THIOACETIC ACID	2.7E-24	4.0E-22	3.1E-21	1.0E-22	3.9E-21	4.7E-20	0.
CYCLOPROP.THIOL	3.2E-20	5.6E-16	3.9E-14	1.2E-15	2.3E-13	2.0E-10	0.
CYCLOBUTA.THIOL	3.2E-26	1.0E-20	4.4E-18	6.9E-20	5.3E-17	2.6E-13	0.
CYCLUPENT.THIOL	2.0E-32	3.8E-23	3.2E-22	2.4E-24	7.8E-21	2.2E-16	0.
CYCLOHEXA.THIOL	2.0E-34	1.2E-23	3.7E-22	1.3E-24	1.8E-20	2.9E-15	0.
M.SULFONIC ACID	1.4E-27	7.9E-28	1.8E-28	4.5E-29	4.4E-29	1.1E-31	0.
E.SULFINIC ACID	6.8E-19	1.7E-16	8.2E-16	1.8E-16	2.1E-15	4.9E-15	0.
THIOPHENE	5.8E-23	1.2E-17	7.5E-15	6.3E-18	2.2E-14	2.8E-09	0.
BENZENETHIOL	7.9E-30	1.0E-21	1.3E-17	5.0E-22	7.4E-17	1.6E-09	0.
THIUGLYCOL	7.5E-26	1.9E-23	9.1E-23	2.0E-23	2.3E-22	5.4E-22	0.
CYSTEINE	5.1E-35	7.6E-32	7.2E-31	1.0E-32	1.2E-30	3.4E-30	0.
METHIONINE	0.	0.	4.3E-38	0.	2.7E-37	2.5E-35	0.

TABLE 40

STANDARD FREE ENERGIES OF FORMATION IN KCAL./MOLE FOR VARIOUS ORGANIC AND INORGANIC COMPOUNDS AT FOUR TEMPERATURES.

## INDEX

Compound Type	First Compound Number
Small Compounds Containing C, H, and O	1
Aliphatic Hydrocarbons	10
Aromatic Hydrocarbons	74
Compounds Containing C, H, and O	86
Compounds Containing N in Addition to C, and H	141
Compounds Containing N in Addition to C, H, and O	191
Amino Acids Containing N, C, H, and O	223
Nucleic Acids and Related Compounds	250
Compounds Containing P and C, H, O or N	260
Compounds Containing S and C, H, O, N or P	272
Compounds Containing Cl	324

TABLE 40  
STANDARD FREE ENERGIES OF FORMATION IN KCAL/MOLE FOR VARIOUS ORGANIC AND INORGANIC  
COMPOUNDS AT FOUR TEMPERATURES.

No.	Compound	Formula	Standard free energies of formation				Ref.
			300°K	500°K	700°K	1000°K	
1	Oxygen, diatomic	O <sub>2</sub>	0.00	0.00	0.00	0.00	a
2	Ozone	O <sub>3</sub>	39.03	42.35	45.67	50.60	b
3	Hydrogen, diatomic	H <sub>2</sub>	0.00	0.00	0.00	0.00	a
4	Water	H <sub>2</sub> O	-54.61	-52.36	-49.92	-46.04	b
5	Hydrogen peroxide	H <sub>2</sub> O <sub>2</sub>	-29.69	-27.39	-25.07	-21.57	c
6	Graphite	C	0.00	0.00	0.00	0.00	a
7	Carbon monoxide	CO	-32.85	-37.18	-41.53	-47.94	a
8	Carbon dioxide	CO <sub>2</sub>	-94.26	-94.39	-94.50	-94.61	a
9	Carbon suboxide	C <sub>3</sub> O <sub>2</sub>	-10.74	-12.49	-14.36	-17.18	b
10	Methane	CH <sub>4</sub>	-12.11	-7.84	-3.05	4.61	a
11	Acetylene	C <sub>2</sub> H <sub>2</sub>	49.98	47.20	44.50	40.60	a
12	Ethylene	C <sub>2</sub> H <sub>4</sub>	16.31	19.25	22.68	28.25	a
13	Ethane	C <sub>2</sub> H <sub>6</sub>	-7.79	1.17	10.90	26.13	a
14	Allene	C <sub>3</sub> H <sub>4</sub>	48.38	50.33	52.68	56.50	a
15	Cyclopropane	C <sub>3</sub> H <sub>6</sub>	21.68	31.20	40.84	55.54	d
16	Cyclobutane	C <sub>4</sub> H <sub>8</sub>	12.41	28.21	44.10	68.15	d
17	Cyclopentane	C <sub>5</sub> H <sub>10</sub>	9.40	29.25	50.52	83.38	a
18	Cyclohexane	C <sub>6</sub> H <sub>12</sub>	7.81	34.07	61.85	104.30	a
19	Propyne	C <sub>3</sub> H <sub>4</sub>	46.48	48.22	50.36	53.95	a
20	Butyne	C <sub>4</sub> H <sub>6</sub>	47.91	54.64	61.57	72.34	d
21	Pentyne	C <sub>5</sub> H <sub>8</sub>	50.01	61.70	73.59	91.80	d
22	Hexyne	C <sub>6</sub> H <sub>10</sub>	52.11	68.75	85.65	111.47	d
23	Heptyne	C <sub>7</sub> H <sub>12</sub>	54.21	75.82	97.69	131.00	d
24	Octyne	C <sub>8</sub> H <sub>14</sub>	56.30	82.86	109.72	150.59	d
25	Nonyne	C <sub>9</sub> H <sub>16</sub>	58.40	89.92	121.76	170.12	d
26	Decyne	C <sub>10</sub> H <sub>18</sub>	60.50	96.97	133.80	189.72	d
27	Hendecyne	C <sub>11</sub> H <sub>20</sub>	62.59	104.02	145.87	209.45	d
28	Dodecyne	C <sub>12</sub> H <sub>22</sub>	64.69	111.08	157.91	228.98	d
29	Tridecyne	C <sub>13</sub> H <sub>24</sub>	66.79	118.13	169.95	248.58	d

TABLE 40 (continued)  
Standard Free Energies of Formation

No.	Compound	Formula	300°K	500°K	700°K	1000°K	Ref.
30	Tetradecyne	C <sub>14</sub> H <sub>26</sub>	68.88	125.18	181.98	268.10	d
31	Pentadecyne	C <sub>15</sub> H <sub>28</sub>	70.98	132.24	194.04	287.77	d
32	Hexadecyne	C <sub>16</sub> H <sub>30</sub>	73.08	139.29	206.08	307.37	d
33	Heptadecyne	C <sub>17</sub> H <sub>32</sub>	75.18	146.35	218.12	326.90	d
34	Octadecyne	C <sub>18</sub> H <sub>34</sub>	77.27	153.39	230.17	346.56	d
35	Nonadecyne	C <sub>19</sub> H <sub>36</sub>	79.37	160.46	242.21	366.09	d
36	Eicosyne	C <sub>20</sub> H <sub>38</sub>	81.47	167.51	254.25	385.69	d
37	Propene	C <sub>3</sub> H <sub>6</sub>	15.05	22.45	30.59	43.43	a
38	Butene	C <sub>4</sub> H <sub>8</sub>	16.50	29.12	41.96	61.65	d
39	Pentene	C <sub>5</sub> H <sub>10</sub>	18.60	36.18	53.98	81.11	d
40	Hexene	C <sub>6</sub> H <sub>12</sub>	20.69	43.22	66.03	100.77	d
41	Heptene	C <sub>7</sub> H <sub>14</sub>	22.79	50.28	78.07	120.30	d
42	Octene	C <sub>8</sub> H <sub>16</sub>	24.89	57.34	90.13	139.97	d
43	Nonene	C <sub>9</sub> H <sub>18</sub>	26.99	64.39	102.17	159.57	d
44	Decene	C <sub>10</sub> H <sub>20</sub>	29.08	71.44	114.22	179.16	d
45	Hendecene	C <sub>11</sub> H <sub>22</sub>	31.18	78.49	126.26	198.76	d
46	Dodecene	C <sub>12</sub> H <sub>24</sub>	33.28	85.56	138.30	218.29	d
47	Tridecene	C <sub>13</sub> H <sub>26</sub>	35.37	92.60	150.35	237.95	d
48	Tetradecene	C <sub>14</sub> H <sub>28</sub>	37.47	99.65	162.39	257.55	d
49	Pentadecene	C <sub>15</sub> H <sub>30</sub>	39.57	106.71	174.43	277.08	d
50	Hexadecene	C <sub>16</sub> H <sub>32</sub>	41.66	113.76	186.48	296.74	d
51	Heptadecene	C <sub>17</sub> H <sub>34</sub>	43.76	120.82	198.52	316.27	d
52	Octadecene	C <sub>18</sub> H <sub>36</sub>	45.86	127.87	210.58	335.94	d
53	Nonadecene	C <sub>19</sub> H <sub>38</sub>	47.96	134.93	220.60	355.40	d
54	Eicosene	C <sub>20</sub> H <sub>40</sub>	50.05	141.98	234.65	375.06	d
55	Propane	C <sub>3</sub> H <sub>8</sub>	-5.54	8.23	22.93	45.68	a
56	Butane	C <sub>4</sub> H <sub>10</sub>	-3.94	14.54	34.19	64.50	a
57	Isobutane	C <sub>4</sub> H <sub>10</sub>	-4.83	14.39	34.74	66.09	a
58	Pentane	C <sub>5</sub> H <sub>12</sub>	-1.80	21.51	46.20	84.18	a
59	Hexane	C <sub>6</sub> H <sub>14</sub>	0.18	28.30	57.98	103.57	a
60	Heptane	C <sub>7</sub> H <sub>16</sub>	2.23	35.14	69.83	123.05	a
61	Octane	C <sub>8</sub> H <sub>18</sub>	4.29	42.02	81.74	142.62	a
62	Nonane	C <sub>9</sub> H <sub>20</sub>	6.34	48.90	93.95	162.18	a
63	Decane	C <sub>10</sub> H <sub>22</sub>	8.39	55.79	105.56	181.75	a
64	Hendecane	C <sub>11</sub> H <sub>24</sub>	10.44	62.67	117.47	201.31	a
65	Dodecane	C <sub>12</sub> H <sub>26</sub>	12.50	69.55	129.38	220.88	a

TABLE 40 (continued)

## Standard Free Energies of Formation

No.	Compound	Formula	300°K	500°K	700°K	1000°K	Ref.
66	Tridecane	C <sub>13</sub> H <sub>28</sub>	14.55	76.43	141.29	240.45	a
67	Tetradecane	C <sub>14</sub> H <sub>30</sub>	16.60	83.31	153.20	260.01	a
68	Pentadecane	C <sub>15</sub> H <sub>32</sub>	18.66	90.20	165.11	279.58	a
69	Hexadecane	C <sub>16</sub> H <sub>34</sub>	20.71	97.08	177.02	299.14	a
70	Heptadecane	C <sub>17</sub> H <sub>36</sub>	22.76	103.96	188.93	318.71	a
71	Octadecane	C <sub>18</sub> H <sub>38</sub>	24.82	110.84	200.84	338.28	a
72	Nonadecane	C <sub>19</sub> H <sub>40</sub>	26.87	117.72	212.75	357.84	a
73	Eicosane	C <sub>20</sub> H <sub>42</sub>	28.92	124.61	224.66	377.41	a
74	Benzene	C <sub>6</sub> H <sub>6</sub>	31.06	39.24	48.21	62.27	a
75	Toluene	C <sub>7</sub> H <sub>8</sub>	29.34	41.81	55.31	76.32	a
76	Xylene	C <sub>8</sub> H <sub>10</sub>	29.10	46.72	65.60	94.90	a
77	Ethylbenzene	C <sub>8</sub> H <sub>10</sub>	31.36	48.55	66.92	95.30	a
78	Azulene	C <sub>10</sub> H <sub>8</sub>	55.85	68.03	81.18	102.07	d
79	Diethylbenzene	C <sub>10</sub> H <sub>14</sub>	32.25	60.90	89.55	132.53	d
80	Biphenyl	C <sub>12</sub> H <sub>10</sub>	66.00	83.29	100.90	127.92	d
81	Naphthalene	C <sub>10</sub> H <sub>8</sub>	56.27	68.72	81.17	99.85	d
82	Benzonaphthalene	C <sub>13</sub> H <sub>10</sub>	79.43	100.71	122.31	155.31	d
83	Anthracene	C <sub>14</sub> H <sub>10</sub>	82.35	100.23	118.49	146.58	d
84	Trimethylnaphthalene	C <sub>17</sub> H <sub>16</sub>	78.33	111.23	144.15	193.55	d
85	Asphalt	C <sub>22</sub> H <sub>12</sub>	137.40	160.68	183.96	218.88	d
86	Ethylene oxide	C <sub>2</sub> H <sub>4</sub> O	-2.77	4.52	11.85	22.91	d
87	Propylene oxide	C <sub>3</sub> H <sub>6</sub> O	-5.49	6.18	18.60	37.74	f
88	Acetone	C <sub>3</sub> H <sub>6</sub> O	-36.20	-25.20	-13.40	4.91	e
89	Ketene	C <sub>2</sub> H <sub>2</sub> O	-13.22	-12.35	-11.46	-10.08	d
90	Furan	C <sub>4</sub> H <sub>4</sub> O	0.26	6.45	13.16	23.60	k
91	Phenol	C <sub>6</sub> H <sub>6</sub> O	-7.79	2.96	14.34	31.82	i
92	Benzoic acid	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	-57.23	-43.09	-28.77	-6.97	d
93	Methanol	CH <sub>4</sub> O	-39.00	-32.05	-25.14	-14.85	d
94	Ethanol	C <sub>2</sub> H <sub>6</sub> O	-39.91	-28.47	-16.39	2.19	s
95	Octanol	C <sub>8</sub> H <sub>18</sub> O	-27.34	14.48	56.60	120.36	d
96	Octadecanol	C <sub>18</sub> H <sub>38</sub> O	-6.37	85.02	177.03	316.19	d
97	Formaldehyde	CH <sub>2</sub> O	-26.26	-25.07	-23.57	-21.02	b
98	Acetaldehyde	C <sub>2</sub> H <sub>4</sub> O	-31.71	-25.97	-19.69	-9.81	h
99	Formic acid	CH <sub>2</sub> O <sub>2</sub>	-83.85	-79.16	-74.20	-66.53	j
100	Acetic acid	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-94.11	-83.80	-73.37	-57.50	d

TABLE 40 (continued)  
Standard Free Energies of Formation

No.	Compound	Formula	300°K	500°K	700°K	1000°K	Ref.
101	Acetic anhydride	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	-77.64	-66.58	-55.36	-38.23	d
102	Propionic acid	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-92.01	-76.74	-61.33	-37.97	d
103	Butyric acid	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-89.91	-69.68	-49.27	-18.30	d
104	Octanoic acid	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	-81.53	-42.21	-2.91	56.02	d
105	Nonanoic acid	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	-79.43	-34.41	10.93	79.54	d
106	Nonadecanoic acid	C <sub>19</sub> H <sub>38</sub> O <sub>2</sub>	-58.46	36.13	131.38	275.51	d
107	Propenoic acid	C <sub>3</sub> H <sub>4</sub> O <sub>2</sub>	-79.69	-63.29	-46.89	-22.29	d
108	Glyoxalic acid	C <sub>2</sub> H <sub>2</sub> O <sub>3</sub>	-116.75	-110.20	-106.23	-105.13	d
109	Glycolic acid	C <sub>2</sub> H <sub>4</sub> O <sub>3</sub>	-125.43	-112.29	-99.15	-79.44	d
110	Oxalic acid	C <sub>2</sub> H <sub>2</sub> O <sub>4</sub>	-179.21	-168.82	-163.77	-166.20	d
111	Pyruvic acid	C <sub>3</sub> H <sub>4</sub> O <sub>3</sub>	-92.72	-81.96	-71.12	-54.71	d
112	Lactic acid	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	-123.80	-105.10	-86.32	-58.00	d
113	Glyceric acid	C <sub>3</sub> H <sub>6</sub> O <sub>4</sub>	-155.13	-133.48	-111.77	-79.11	d
114	Fumaric acid	C <sub>4</sub> H <sub>4</sub> O <sub>4</sub>	-163.57	-140.42	-117.21	-82.30	d
115	Oxaloacetic acid	C <sub>4</sub> H <sub>4</sub> O <sub>5</sub>	-202.87	-184.57	-166.21	-138.54	d
116	Acetoacetic acid	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	-117.36	-100.54	-83.70	-58.42	d
117	Crotonic acid	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	-78.06	-56.11	-34.04	-0.71	d
118	$\alpha$ -Ketobutyric acid	C <sub>4</sub> H <sub>6</sub> O <sub>3</sub>	-117.36	-100.27	-83.04	-56.95	d
119	Acetoxyacetic acid	C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>	-135.70	-120.58	-105.44	-82.71	d
120	Succinic acid	C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>	-175.43	-154.00	-132.45	-99.90	d
121	Hydroxybutanoic acid	C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>	-121.71	-98.05	-74.25	-38.27	d
122	Citric acid	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>	-289.79	-252.89	-215.97	-160.57	d
123	Palmitic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	-64.75	13.44	91.65	209.02	d
124	Glyoxal	C <sub>2</sub> H <sub>2</sub> O <sub>2</sub>	-53.53	-50.17	-46.81	-41.78	d
125	Glycolaldehyde	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	-62.59	-53.72	-44.73	-31.02	d
126	Glycol	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	-71.66	-55.70	-40.58	-17.93	d
127	Glycerol	C <sub>3</sub> H <sub>8</sub> O <sub>3</sub>	-100.94	-77.52	-54.04	-18.69	d
128	Glyceraldehyde	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	-92.29	-75.04	-57.67	-31.39	d
129	Erythrose	C <sub>4</sub> H <sub>8</sub> O <sub>4</sub>	-121.98	-96.26	-70.54	-31.96	d
130	Deoxyribose	C <sub>5</sub> H <sub>10</sub> O <sub>4</sub>	-108.30	-74.79	-41.34	8.74	d
131	Ribose	C <sub>5</sub> H <sub>10</sub> O <sub>5</sub>	-151.68	-117.67	-83.54	-32.12	d
132	Glucose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	-181.37	-138.89	-96.41	-32.69	d
133	Fructose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	-185.68	-143.88	-102.08	-39.38	d
134	Methyl acetate	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	-52.29	-43.31	-34.33	-20.86	d
135	Ethyl acetate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	-50.19	-36.35	-22.51	-1.75	d
136	Dimethyl ether	C <sub>2</sub> H <sub>6</sub> O	-26.53	-18.83	-10.97	1.11	d

TABLE 40 (continued)

## Standard Free Energies of Formation

No.	Compound	Formula	300°K	500°K	700°K	1000°K	Ref.
137	Octylmethyl ether	C <sub>9</sub> H <sub>20</sub> O	-12.26	29.86	72.36	136.84	d
138	18-Methyl ether	C <sub>19</sub> H <sub>40</sub> O	8.71	100.39	192.81	332.81	d
139	Nonylmethyl ester	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	-37.61	6.33	50.65	117.86	d
140	19-Methyl ester	C <sub>20</sub> H <sub>40</sub> O <sub>2</sub>	-16.64	76.86	171.10	313.83	d
141	Nitrogen, diatomic	N <sub>2</sub>	0.00	0.00	0.00	0.00	a
142	Nitric oxide	NO	20.69	20.10	19.49	18.59	b
143	Nitrogen dioxide	NO <sub>2</sub>	12.38	15.37	18.41	22.97	b
144	Nitrogen trioxide	NO <sub>3</sub>	27.81	35.11	42.42	53.23	b
145	Nitrous oxide	N <sub>2</sub> O	24.93	28.51	32.10	37.39	b
146	Nitrous anhydride	N <sub>2</sub> O <sub>3</sub>	33.41	42.53	51.64	65.13	b
147	Nitrogen tetroxide	N <sub>2</sub> O <sub>4</sub>	23.62	37.91	52.13	73.15	b
148	Nitric anhydride	N <sub>2</sub> O <sub>5</sub>	28.34	45.42	62.26	87.03	b
149	Ammonia	NH <sub>3</sub>	-3.94	1.11	6.51	14.93	b
150	Hydrazine	N <sub>2</sub> H <sub>4</sub>	38.11	48.75	59.77	76.49	b
151	Cyanogen	C <sub>2</sub> N <sub>2</sub>	71.10	69.13	67.02	63.78	b
152	Tricyanotriazine	C <sub>6</sub> N <sub>6</sub>	155.16	163.70	172.10	184.47	d
153	Hydroxylamine	NH <sub>3</sub> O	-26.77	-18.83	-10.23	3.89	d
154	Nitrous acid	HNO <sub>2</sub>	-10.46	-4.74	1.07	9.77	b
155	Nitric acid	HNO <sub>3</sub>	-17.60	-7.74	2.26	17.20	b
156	Hydrogen cyanide	HCN	28.69	27.04	25.43	23.07	b
157	Cyanamide	CH <sub>2</sub> N <sub>2</sub>	39.54	43.48	48.08	56.20	d
158	Imidazole	C <sub>3</sub> H <sub>4</sub> N <sub>2</sub>	51.74	64.07	76.46	95.14	d
159	Adenine	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>	111.52	136.34	161.74	200.91	d
160	Pyrrole	C <sub>4</sub> H <sub>5</sub> N	42.39	54.16	66.05	84.10	d
161	Pyridine	C <sub>5</sub> H <sub>5</sub> N	45.54	54.18	63.47	77.79	g
162	Piperidine	C <sub>5</sub> H <sub>11</sub> N	33.31	64.21	95.11	141.45	d
163	Pyrimidine	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub>	49.28	59.00	68.74	83.36	d
164	Purine	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub>	97.34	116.15	134.94	163.07	d
165	Benzonitrile	C <sub>7</sub> H <sub>5</sub> N	61.59	68.79	76.17	87.55	d
166	Phenylisocyanide	C <sub>7</sub> H <sub>5</sub> N	76.65	83.51	90.55	101.42	d
167	Aniline	C <sub>6</sub> H <sub>7</sub> N	43.95	57.98	72.85	96.72	d
168	Quinoline	C <sub>9</sub> H <sub>7</sub> N	65.19	78.08	90.95	110.20	d
169	Azobenzene	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub>	94.93	114.01	134.05	164.92	d
170	Melaniline	C <sub>13</sub> H <sub>13</sub> N <sub>3</sub>	145.56	188.53	231.70	296.83	d
171	Sym-Triazine	C <sub>3</sub> N <sub>3</sub> N <sub>3</sub>	59.70	70.70	81.64	97.97	d
172	Aminotriazine	C <sub>3</sub> H <sub>4</sub> N <sub>4</sub>	73.22	89.80	106.92	133.62	d

TABLE 40 (continued)  
Standard Free Energies of Formation

No.	Compound	Formula	300°K	500°K	700°K	1000°K	Ref.
173	Diaminotriazine	C <sub>3</sub> H <sub>5</sub> N <sub>5</sub>	87.40	109.98	133.74	171.60	d
174	Triaminotriazine	C <sub>3</sub> H <sub>6</sub> N <sub>6</sub>	102.24	131.26	162.08	211.70	d
175	Ethylhydrazine	C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>	31.16	52.39	74.36	108.72	d
176	Methylcyanide	C <sub>2</sub> H <sub>3</sub> N	24.29	27.41	30.61	35.56	d
177	Methylisocyanide	C <sub>2</sub> H <sub>3</sub> N	39.35	42.13	44.99	49.43	d
178	Methylamine	CH <sub>5</sub> N	6.65	16.59	27.27	44.66	d
179	Dimethylamine	C <sub>2</sub> H <sub>7</sub> N	13.81	29.25	44.85	68.55	d
180	Trimethylamine	C <sub>3</sub> H <sub>9</sub> N	18.03	39.35	60.89	93.63	d
181	Ethyleneimine	C <sub>2</sub> H <sub>5</sub> N	29.65	38.14	47.37	62.62	d
182	Ethenylamine	C <sub>2</sub> H <sub>5</sub> N	40.93	51.09	61.35	76.91	d
183	Ethylamine	C <sub>2</sub> H <sub>7</sub> N	8.75	23.65	39.31	64.21	d
184	Octylamine	C <sub>8</sub> H <sub>19</sub> N	21.33	65.97	111.59	181.84	d
185	Octadecylamine	C <sub>18</sub> H <sub>39</sub> N	42.30	136.52	232.00	377.60	d
186	Diaminoethane	C <sub>2</sub> H <sub>8</sub> N <sub>2</sub>	26.09	46.77	68.83	104.49	d
187	Guanidine	CH <sub>5</sub> N <sub>3</sub>	57.88	82.52	108.30	149.08	d
188	Guanylhydrazine	CH <sub>6</sub> N <sub>4</sub>	79.88	110.56	142.38	192.23	d
189	Dicyanodiamide	C <sub>2</sub> H <sub>4</sub> N <sub>4</sub>	97.52	121.37	145.72	183.20	d
190	Melamine	C <sub>3</sub> H <sub>6</sub> N <sub>6</sub>	101.17	129.48	159.59	208.13	d
191	Cyanic acid	HNCO	-25.67	-24.09	-22.42	-19.81	b
192	Nitromethane	CH <sub>3</sub> NO <sub>2</sub>	-1.56	9.77	21.56	39.52	t
193	Methylnitrate	CH <sub>3</sub> NO <sub>3</sub>	-20.54	-10.32	0.32	17.05	d
194	Dinitromethane	CH <sub>2</sub> N <sub>2</sub> O <sub>4</sub>	6.30	26.67	47.35	79.71	d
195	Trinitromethane	CHN <sub>3</sub> O <sub>6</sub>	14.33	43.31	72.70	118.78	d
196	Tetranitromethane	CN <sub>4</sub> O <sub>8</sub>	21.56	60.73	99.70	160.55	d
197	Nitroethane	C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	-0.10	16.78	34.12	61.01	d
198	Methoxyamine	CH <sub>5</sub> NO	-24.67	-11.76	1.81	23.42	d
199	Urea	CH <sub>4</sub> N <sub>2</sub> O	-3.04	9.84	23.98	47.56	d
200	Hydroxyurea	CH <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	-29.71	-13.63	3.11	29.44	d
201	Aminourea	CH <sub>5</sub> N <sub>3</sub> O	18.96	37.88	58.06	90.71	d
202	Diurea	C <sub>2</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	32.91	58.64	84.41	123.14	d
203	Formamide	CH <sub>3</sub> NO	-17.02	-8.73	-3.10	0.34	d
204	Acetamide	C <sub>2</sub> H <sub>5</sub> NO	-18.70	-7.01	4.62	21.97	d
205	Oxamide	C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	-28.80	-14.38	1.30	27.20	d
206	Dicyanodiamidine	C <sub>2</sub> H <sub>6</sub> N <sub>4</sub> O	54.53	87.03	120.67	173.25	d
207	Ethanolamine	C <sub>2</sub> H <sub>7</sub> NO	-22.58	-4.72	13.86	43.08	d

TABLE 40 (continued)

## Standard Free Energies of Formation

No.	Compound	Formula	300°K	500°K	700°K	1000°K	Ref.
208	$\alpha$ -Ethylhydroxylamine	C <sub>2</sub> H <sub>7</sub> NO	-9.59	3.62	17.57	39.90	d
209	$\beta$ -Ethylhydroxylamine	C <sub>2</sub> H <sub>7</sub> NO	-17.51	0.88	19.39	47.38	d
210	Cyanuric acid	C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>3</sub>	-43.76	-23.23	-2.80	27.69	d
211	Ammelide	C <sub>3</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	3.84	26.49	49.66	85.39	d
212	Ammeline	C <sub>3</sub> H <sub>5</sub> N <sub>5</sub> O	52.50	77.98	104.64	146.86	d
213	Nitrobenzene	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	35.10	51.10	67.66	93.54	d
214	Oxamic acid	C <sub>2</sub> H <sub>3</sub> NO <sub>3</sub>	-104.21	-91.24	-77.61	-55.91	d
215	$\alpha$ -Aminobutyric acid	C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>	-72.57	-46.56	-19.77	21.86	d
216	Uric acid	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>3</sub>	29.89	62.84	95.81	145.32	d
217	Orotic acid	C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>4</sub>	-82.67	-57.43	-32.13	5.95	d
218	Hydroxyglutamic acid	C <sub>5</sub> H <sub>9</sub> NO <sub>5</sub>	-188.24	-152.18	-115.40	-58.88	d
219	Nicotinic acid	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	-47.47	-32.49	-17.43	5.31	d
220	Quinic acid	C <sub>7</sub> H <sub>5</sub> NO <sub>4</sub>	-134.04	-112.69	-91.22	-58.79	d
221	Folic acid	C <sub>19</sub> H <sub>19</sub> N <sub>7</sub> O <sub>6</sub>	-30.62	49.87	131.42	255.75	d
222	Tetrahydroxyfolic acid	C <sub>19</sub> H <sub>23</sub> N <sub>7</sub> O <sub>6</sub>	-26.05	68.88	164.79	310.51	d
223	Glycine	C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	-76.76	-60.66	-43.84	-17.26	d
224	Alanine	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	-75.13	-53.61	-31.35	3.41	d
225	Serine	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	-106.46	-81.98	-56.78	-17.63	d
226	Threonine	C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub>	-104.83	-74.93	-44.29	3.04	d
227	Valine	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	-71.41	-39.50	-6.77	43.88	d
228	Leucine	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	-69.31	-32.45	5.27	63.48	d
229	Aspartic acid	C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub>	-158.55	-130.87	-102.47	-58.52	d
230	Glutamic acid	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	-156.45	-123.82	-90.41	-38.85	d
231	Asparagine	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	-83.14	-54.01	-23.54	24.66	d
232	Glutamine	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	-81.04	-46.95	-11.48	44.33	d
233	Proline	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>	-55.86	-27.94	0.20	42.84	d
234	Histidine	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	-10.64	28.77	68.86	130.27	d
235	Lysine	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	-51.50	-9.32	34.30	102.43	d
236	Arginine	C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>	4.39	61.52	119.91	209.84	d
237	Phenylalanine	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	-36.15	-5.86	25.29	73.61	d
238	Tyrosine	C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	-70.64	-37.17	-2.86	50.18	d
239	Tryptophan	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	2.56	41.38	81.08	142.28	d
240	Glycylglycine	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	-77.61	-48.41	-18.49	27.74	d
241	$\beta$ -Alanine	C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub>	-74.67	-53.61	-31.83	2.19	d
242	$\alpha$ -Hydroxyalanine	C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub>	-107.71	-82.18	-56.05	-15.73	d
243	Hydroxylysine	C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	-83.29	-37.68	9.31	82.40	d

TABLE 40 (continued)

## Standard Free Energies of Formation

No.	Compound	Formula	300°K	500°K	700°K	1000°K	Ref.
244	Ornithine	C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	-53.59	-16.37	22.27	82.91	d
245	Creatine	C <sub>4</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	-14.57	27.31	69.85	134.88	d
246	Hydroxyproline	C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub>	-87.65	-56.32	-24.77	22.95	d
247	Formylglycine	C <sub>3</sub> H <sub>5</sub> NO <sub>3</sub>	-92.27	-73.88	-55.37	-27.38	d
248	Acetylglycine	C <sub>4</sub> H <sub>7</sub> NO <sub>3</sub>	-94.95	-71.54	-47.99	-12.42	d
249	Dimethylglycine	C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub>	-65.39	-37.92	-10.23	31.70	d
250	Uracil	C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	3.90	22.77	41.68	70.12	d
251	Cytosine	C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O	40.57	60.73	81.55	114.00	d
252	Thymine	C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	2.84	26.87	51.04	87.54	d
253	Guanine	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O	89.04	118.57	148.70	195.02	d
254	Inosine	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>	-19.01	40.21	99.33	187.84	d
255	Xanthine	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	52.37	80.61	108.85	151.21	d
256	Hypoxanthine	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O	74.85	98.38	121.87	157.03	d
257	Nitroguanidine	CH <sub>4</sub> N <sub>4</sub> O <sub>2</sub>	71.03	103.68	137.19	189.05	d
258	Nicotinamide	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O	27.94	44.36	61.52	88.63	d
259	Pyridoxal	C <sub>8</sub> H <sub>9</sub> NO <sub>3</sub>	-52.57	-25.51	1.77	43.12	d
260	Phosphorus, monatomic	P	54.51	51.93	49.23	45.09	b
261	Phosphorus, diatomic	P <sub>2</sub>	0.00	0.00	0.00	0.00	a
262	Phosphorus, tetratomic	P <sub>4</sub>	2.01	-36.00	-28.70	-18.01	b
263	Phosphorus monohydride	PH	36.19	35.24	34.26	32.84	b
264	Phosphorus dihydride	PH <sub>2</sub>	5.95	4.13	2.12	-1.16	b
265	Phosphine	PH <sub>3</sub>	-9.15	-4.28	0.82	8.64	b
266	Phosphorus monocarbide	PC	83.01	78.19	73.28	65.97	b
267	Phosphorus mononitride	PN	3.18	2.96	2.69	2.65	b
268	Phosphorus monoxide	PO	-23.66	-24.14	-24.68	-25.58	b
269	Phosphorus dioxide	PO <sub>2</sub>	-88.08	-85.08	-82.15	-77.81	b
270	Phosphorus trioxide, dimeric	P <sub>4</sub> O <sub>6</sub>	-547.59	-513.67	-480.45	-431.61	b
271	Phosphorus pentoxide, dimeric	P <sub>4</sub> O <sub>10</sub>	-683.71	-631.90	-580.67	-504.97	b
272	Sulfur, monatomic	S	46.39	43.73	40.96	36.72	b
273	Sulfur, diatomic	S <sub>2</sub>	0.00	0.00	0.00	0.00	a
274	Sulfur, octatomic	S <sub>8</sub>	-65.12	-41.82	-19.93	12.12	b
275	Sulfur monohydride	SH	15.33	14.63	13.86	12.73	b
276	Hydrogen sulfide	H <sub>2</sub> S	-17.44	-15.43	-13.43	-9.78	b
277	Sulfur mononitride	SN	46.62	46.11	45.50	44.55	b

TABLE 40 (continued)  
Standard Free Energies of Formation

No.	Compound	Formula	300°K	500°K	700°K	1000°K	Ref.
278	Phosphorus monosulfide	PS	-15.33	-15.65	-16.26	-17.21	b
279	Sesquisulfide	P <sub>4</sub> S <sub>3</sub>	-118.66	-96.70	-75.91	-45.81	b
280	Sulfur monoxide	SO	-15.08	-15.52	-15.76	-16.12	b
281	Sulfur dioxide	SO <sub>2</sub>	-81.28	-77.82	-74.32	-69.07	b
282	Sulfur trioxide	SO <sub>3</sub>	-98.04	-90.08	-82.13	-70.38	b
283	Carbon monosulfide	CS	32.99	28.70	24.31	17.79	b
284	Carbon disulfide	CS <sub>2</sub>	-3.32	-3.39	-3.68	-4.16	b
285	Carbon oxysulfide	COS	-49.25	-49.63	-50.12	-50.86	b
286	Sulfurous acid	H <sub>2</sub> SO <sub>3</sub>	-95.46	-83.56	-71.66	-53.81	d
287	Sulfuric acid	H <sub>2</sub> SO <sub>4</sub>	-141.28	-125.13	-109.48	-86.96	d
288	Methanethiol	CH <sub>4</sub> S	-11.86	-5.43	1.48	12.23	m
289	Ethanethiol	C <sub>2</sub> H <sub>6</sub> S	-10.56	0.59	12.40	30.59	m
290	Octanethiol	C <sub>8</sub> H <sub>18</sub> S	2.91	44.31	86.01	149.14	d
291	Octadecanethiol	C <sub>18</sub> H <sub>38</sub> S	23.88	114.85	206.44	344.97	d
292	Benzanethiol	C <sub>6</sub> H <sub>6</sub> S	25.80	36.09	47.00	63.75	r
293	Cyclopropanethiol	C <sub>3</sub> H <sub>6</sub> S	13.37	20.09	27.31	38.46	u
294	Cyclobutanethiol	C <sub>4</sub> H <sub>8</sub> S	16.43	28.51	41.39	61.20	o
295	Cyclopentanethiol	C <sub>5</sub> H <sub>10</sub> S	4.28	26.18	49.33	84.82	p
296	Cyclohexanethiol	C <sub>6</sub> H <sub>12</sub> S	3.47	27.16	51.90	89.28	l
297	Dimethylsulfide	C <sub>2</sub> H <sub>6</sub> S	-7.77	3.86	16.17	35.10	m
298	Dimethyldisulfide	C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>	-15.43	-0.84	14.32	37.38	m
299	Diethylsulfide	C <sub>4</sub> H <sub>10</sub> S	-5.10	16.01	38.18	72.08	m
300	Diethyldisulfide	C <sub>4</sub> H <sub>10</sub> S <sub>2</sub>	-13.54	10.69	35.80	73.97	m
301	Ethanedithiol	C <sub>2</sub> H <sub>6</sub> S <sub>2</sub>	-10.75	3.45	17.71	39.23	d
302	Thiophene	C <sub>4</sub> H <sub>4</sub> S	20.62	26.72	33.24	43.26	n
303	3-Methylthiophene	C <sub>5</sub> H <sub>6</sub> S	19.80	30.57	41.99	59.53	q
304	Cyanogensulfide	C <sub>2</sub> N <sub>2</sub> S	58.53	58.83	59.15	59.64	d
305	Thioformic acid	CH <sub>2</sub> SO	-18.64	-14.96	-11.28	-5.76	d
306	Thioacetic acid	C <sub>2</sub> H <sub>4</sub> SO	-21.32	-13.72	-2.94	19.21	d
307	Methylsulfonic acid	CH <sub>3</sub> SO <sub>3</sub>	-107.86	-89.81	-71.78	-44.79	d
308	Methylbisulfate	CH <sub>3</sub> SO <sub>4</sub>	-126.20	-109.85	-93.52	-69.08	d
309	Ethylsulfinic acid	C <sub>2</sub> H <sub>6</sub> SO	-74.44	-54.39	-34.28	-4.02	d
310	Ethylsulfonic acid	C <sub>2</sub> H <sub>6</sub> SO <sub>3</sub>	-105.76	-82.75	-59.72	-25.12	d
311	Ethylsulfuric acid	C <sub>2</sub> H <sub>6</sub> SO <sub>4</sub>	-124.10	-102.79	-81.46	-49.41	d
312	Methylsulfite	C <sub>2</sub> H <sub>6</sub> SO <sub>3</sub>	-65.30	-52.80	-40.14	-20.85	d
313	Methylsulfate	C <sub>2</sub> H <sub>6</sub> SO <sub>4</sub>	-111.12	-94.47	-77.76	-52.60	d

TABLE 40 (continued)  
Standard Free Energies of Formation

No.	Compound	Formula	300°K	500°K	700°K	1000°K	Ref.
314	Carbylsulfate	C <sub>2</sub> H <sub>4</sub> S <sub>2</sub> O <sub>6</sub>	-170.20	-145.01	-119.92	-82.49	d
315	Thioglycol	C <sub>2</sub> H <sub>6</sub> SO	-28.61	-12.72	3.35	27.81	d
316	Thiocyanic acid	HNCS	21.12	21.82	22.52	23.57	d
317	Purinethiol	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> S	93.10	114.67	136.20	168.42	d
318	Methylthiocyanate	C <sub>2</sub> H <sub>3</sub> NS	25.33	31.25	37.35	46.65	d
319	Aminoethanethiol	C <sub>2</sub> H <sub>7</sub> NS	7.67	25.11	43.27	71.86	d
320	Trithiocyanuric acid	C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> S <sub>3</sub>	46.98	65.26	85.40	113.88	d
321	Cysteine	C <sub>3</sub> H <sub>7</sub> NSO <sub>2</sub>	-76.21	-52.15	-27.37	11.15	d
322	Methionine	C <sub>5</sub> H <sub>11</sub> NSO <sub>2</sub>	-70.00	-35.66	-0.50	53.76	d
323	Mesocystine	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> S <sub>2</sub> O <sub>4</sub>	-135.60	-85.95	-34.88	44.37	d
324	Chlorine, diatomic	Cl <sub>2</sub>	0.00	0.00	0.00	0.00	a
325	Chlorine monoxide	ClO	23.29	22.69	22.07	21.12	b
326	Chlorine dioxide	ClO <sub>2</sub>	29.26	32.14	35.02	39.31	b
327	Dichlorine monoxide	Cl <sub>2</sub> O	22.34	25.20	28.06	32.33	b
328	Hydrogen chloride	HCl	-22.69	-23.13	-23.51	-24.00	b
329	Hydrogen oxychloride	HOCl	-18.94	-16.79	-14.52	-11.00	b
330	Carbonyl chloride	COCl <sub>2</sub>	-49.20	-46.95	-44.73	-41.44	b
331	Carbon tetrachloride	CCl <sub>4</sub>	-15.77	-9.10	-2.61	6.90	b
332	Trichloromethane	CHCl <sub>3</sub>	-17.13	-11.80	-6.41	1.67	b
333	Dichloromethane	CH <sub>2</sub> Cl <sub>2</sub>	-16.02	-11.52	-6.75	0.59	b
334	Chloromethane	CH <sub>3</sub> Cl	-14.93	-10.77	-6.18	1.07	b
335	Cyanogen chloride	CNCI	30.53	29.37	28.14	26.27	b
336	Nitrosyl chloride	NOCl	16.07	18.38	20.67	24.06	b
337	Nitryl chloride	NO <sub>2</sub> Cl	16.36	23.13	29.90	39.95	b
338	Phosphorus trichloride	PCl <sub>3</sub>	-74.49	-68.21	-62.14	-53.30	b
339	Phosphorus pentachloride	PCl <sub>5</sub>	-81.65	-67.32	-53.37	-32.91	b
340	Phosphoryl chloride	POCl <sub>3</sub>	-135.23	-124.69	-114.38	-99.22	b
341	Thiophosphoryl chloride	PSCl <sub>3</sub>	-107.93	-97.36	-87.15	-72.16	b

a Rossini, F. D., Pitzer, K. S., Arnett, R. L., Braun, R. M. and Pimentel, G. C., "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds", American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh (1953). The values for all the compounds are based with reference to zero values at all temperatures for diatomic molecules.

b "JANAF Thermochemical Data", prepared under the auspices of the Joint Army-Navy-Air Force Thermochemical Panel at the Thermal Laboratory, the Dow Chemical Company, Midland, Michigan. Dr. Stull, Daniel R., Project Director. (1965)

TABLE 40 (continued)

- c "Selected Values of Chemical Thermodynamic Properties", National Bureau of Standards, U. S. Department of Commerce, Washington, D. C. (1952). Dr. Astin, A. V., Director.
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TABLE 41  
STANDARD FREE ENERGIES OF FORMATION IN KCAL/MOLE FOR VARIOUS GROUPS AT FOUR TEMPERATURES \*

For explanation and examples of the use of this table see pages 172 and table 42.

Group	Standard free energies of formation			
	300°K	500°K	700°K	1000°K
-C-	13.16	20.43	27.55	37.97
-CH	8.02	13.84	19.66	28.39
-CH <sub>2</sub> -	2.10	7.05	12.04	19.59
-CH <sub>3</sub>	-4.30	0.26	4.90	12.00
HC $\begin{smallmatrix} \swarrow \\ \searrow \end{smallmatrix}$	4.89	6.18	7.51	9.55
-C $\begin{smallmatrix} \swarrow \\ \searrow \end{smallmatrix}$	8.13	10.03	11.96	14.88
$\leftrightarrow$ C $\begin{smallmatrix} \swarrow \\ \searrow \end{smallmatrix}$	8.15	9.25	10.37	12.08
$\leftrightarrow$ CH <sub>2</sub>	7.46	8.92	10.43	12.79
$\begin{smallmatrix} \text{H} \\   \end{smallmatrix}$ C $\leftrightarrow$	10.51	12.57	14.66	17.84
>C $\leftrightarrow$	13.67	16.56	19.39	23.49
>C=C<	32.85	38.00	43.15	50.86
$\begin{smallmatrix} \text{H} \\   \end{smallmatrix}$ C=C<	27.10	31.61	36.16	43.09
$\begin{smallmatrix} \text{H} \\ / \end{smallmatrix}$ C=C $\begin{smallmatrix} \backslash \\ \text{H} \end{smallmatrix}$	22.93	26.64	30.46	36.37
$\begin{smallmatrix} \text{H} \\   \end{smallmatrix}$ C=C $\begin{smallmatrix} \text{H} \\ \backslash \end{smallmatrix}$	23.56	27.33	31.22	37.27
H <sub>2</sub> C=C<	22.21	26.12	30.03	35.91
H <sub>2</sub> C=C $\begin{smallmatrix} \text{H} \\ \backslash \end{smallmatrix}$	18.70	21.80	25.01	30.02
H <sub>2</sub> C=C=C $\begin{smallmatrix} \text{H} \\ \backslash \end{smallmatrix}$	52.48	54.59	56.78	60.20
H <sub>2</sub> C=C=C<	55.51	58.45	61.40	65.82
$\begin{smallmatrix} \text{H} \\   \end{smallmatrix}$ C=C=C $\begin{smallmatrix} \text{H} \\ \backslash \end{smallmatrix}$	56.91	59.87	62.84	67.29
HC≡	24.75	23.27	21.81	19.65
-C≡	25.36	24.06	22.81	21.02
Pentene ring	-10.84	-15.26	-19.70	-26.40
Hexene ring	-15.24	-19.28	-23.35	-29.51
3 Ring	14.32	8.25	2.22	-6.77

TABLE 41 (continued)

## Standard Free Energies of Formation

Group		300°K	500°K	700°K	1000°K
4 Ring		2.78	-2.08	-6.97	-14.38
5 Ring		-2.77	-7.63	-12.36	-19.23
6 Ring		-6.03	-9.22	-12.37	-17.00
>C—C<		10.97	9.77	8.54	6.66
>C—C<		-5.07	-4.92	-4.89	-5.06
>C—C<					
-OH		-37.72	-35.16	-32.60	-28.76
-O-		-18.34	-20.04	-21.74	-24.29
		-15.97	-14.68	-13.51	-11.99
-C=O		-26.97	-25.62	-24.19	-21.90
>C=O		-25.35	-23.53	-21.71	-18.98
		-89.81	-84.05	-78.27	-69.55
		-84.79	-79.57	-74.35	-66.52
>N-		30.92	38.56	46.20	57.66
>NH		22.41	28.73	35.05	44.53
-NH <sub>2</sub>		10.95	16.34	22.37	32.62
		14.65	16.79	18.87	21.89
-C≡N		28.59	27.15	25.71	23.55
-N≡C		43.65	41.87	40.09	37.42
-NO <sub>2</sub>		2.10	9.46	17.17	29.39
-SH		-7.47	-5.33	-3.19	0.02
-S-		0.94	3.85	6.75	11.08
		0.56	1.49	2.41	3.76
>SO		-20.02	-13.24	-6.46	3.71
>SO <sub>2</sub>		-65.84	-54.91	-44.08	-28.03
-F		-45.70	-46.10	-46.50	-47.10
-Cl		-8.25	-8.25	-8.25	-8.25

TABLE 41 (continued)

## Standard Free Energies of Formation

Group	300°K	500°K	700°K	1000°K
-Br	-2.40	-2.92	-3.44	-4.22
-I	7.80	7.80	7.80	7.80
Side chain with 2 or more C atoms	1.31	1.31	1.31	1.31
3 Adjacent $\begin{array}{c}   \\ -\text{CH}- \end{array}$ groups	2.12	2.12	2.12	2.12
Adjacent $\begin{array}{c}   \\ -\text{CH}- \end{array}$ and $\begin{array}{c}   \\ -\text{C}- \end{array}$ groups	1.80	1.80	1.80	1.80
2 Adjacent $\begin{array}{c}   \\ -\text{C}- \end{array}$ groups	2.58	2.58	2.58	2.58
Single branching in 5 ring	-1.04	-1.33	-1.55	-1.74
1,1 branching in 5 ring	-1.85	-2.09	-2.35	-2.78
cis 1,2 branching in 5 ring	-0.38	-0.38	-0.38	-0.38
trans 1,2 branching in 5 ring	-2.55	-2.72	-2.99	-3.55
cis 1,3 branching in 5 ring	-1.20	-1.38	-1.61	-2.01
trans 1,3 branching in 5 ring	-2.35	-2.54	-2.82	-3.39
Single branching in 6 ring	-0.93	-1.05	-1.24	-1.65
1,1 branching in 6 ring	-0.27	-1.23	-2.22	-3.79
cis 1,2 branching in 6 ring	-0.19	-0.37	-0.65	-1.23
trans 1,2 branching in 6 ring	-2.41	-2.65	-3.02	-3.85
cis 1,3 branching in 6 ring	-2.70	-2.85	-3.05	-3.46
trans 1,3 branching in 6 ring	-1.60	-1.74	-1.99	-2.57
cis 1,4 branching in 6 ring	-1.11	-1.11	-1.11	-1.11
trans 1,4 branching in 6 ring	-2.80	-2.81	-2.95	-3.37
1,2 branching in aromatics	1.02	1.02	1.02	1.02
1,3 branching in aromatics	-0.31	-0.31	-0.31	-0.31
1,4 branching in aromatics	0.93	0.93	0.93	0.93
1,2,3 branching in aromatics	1.91	1.99	2.06	2.11
1,2,4 branching in aromatics	1.10	1.10	1.10	1.10
1,3,5 branching in aromatics	0.	0.	0.	0.
RT ln2	0.41	0.69	0.97	1.38

TABLE 41 (continued)  
Standard Free Energies of Formation

Group	300°K	500°K	700°K	1000°K
RT 1n3	0.65	1.09	1.53	2.18
RT 1n4	0.83	1.38	1.93	2.76
RT 1n5	0.96	1.60	2.24	3.20
RT 1n6	1.07	1.78	2.49	3.56
RT 1n8	1.24	2.06	2.89	4.13
RT 1n12	1.48	2.49	3.46	4.94
RT 1n24	1.89	3.15	4.42	6.31

↔ Indicates resonant bond in aromatic ring

\* These free energy values were calculated from the equations of van Krevelen and Chermin. (See pages 14 and 15)

TABLE 42

CALCULATIONS OF STANDARD FREE ENERGIES OF FORMATION IN KCAL/MOLE BY THE GROUP CONTRIBUTION METHOD FOR ANTHRACENE, GLYCINE, AND CYCLOHEXANE.

(A description of the method is given on pages 14 and 15.  
Results of other computations are given in Table 41.)

Anthracene:  $C_{14}H_{10}$

$\sigma = 4$

Group	No. of groups	Free energies of formation			
		300°K	500°K	700°K	1000°K
$HC \begin{smallmatrix} \swarrow \\ \uparrow \\ \searrow \end{smallmatrix}$	10	48.90	61.80	75.10	95.50
$\begin{smallmatrix} \leftrightarrow \\ \leftarrow \end{smallmatrix} C \begin{smallmatrix} \swarrow \\ \uparrow \\ \searrow \end{smallmatrix}$	4	32.60	37.00	41.48	48.32
RT lnσ	1	0.83	1.38	1.93	2.76
Total		82.33	100.18	118.51	146.58

Glycine:  $C_2H_5NO_2$

Group	No. of groups	Free energies of formation			
		300°K	500°K	700°K	1000°K
$-CH_2-$	1	2.10	7.05	12.04	19.59
$\begin{smallmatrix} -NH_2 \\ O \\ -C-OH \end{smallmatrix}$	1	10.95	16.34	22.37	32.62
Total		-89.81	-84.05	-78.27	-69.55
		-76.76	-60.66	-43.86	-17.34

Cyclohexane:  $C_6H_{12}$

$\sigma = 6$

Group	No. of groups	Free energies of formation			
		300°K	500°K	700°K	1000°K
$-CH_2-$	6	12.60	42.30	72.24	117.54
6 Ring	1	-6.03	-9.22	-12.37	-17.00
RT lnσ	1	1.07	1.78	2.49	3.56
Total		7.64	34.86	62.36	104.10

**Chapter 2**  
**Description of**  
**Computational Methods**

## CHAPTER 2

### DESCRIPTION OF COMPUTATIONAL METHODS

#### Gibbs Free Energy Function

In the quantitative treatment\* of chemical equilibrium in ideal gas systems at constant pressure and temperature it is convenient to use the Gibbs free energy function, F:

$$F = E + PV - TS$$

$$\text{or } F = H - TS$$

where  
E = internal energy  
H = enthalpy  
S = entropy  
P = pressure  
V = volume  
T = temperature

The case of ideal gas mixtures is particularly easy to treat, as the total free energy of such a system is the sum of the free energies of the constituents each taken separately, at its own partial pressure. The total free energy function properly combines the opposing effects on equilibrium of the pressure or concentration of a compound and its internal energy. The concentration of compounds that are unstable relative to their stoichiometric breakdown products will be small, but not zero.

The elements will distribute themselves among compounds in such a way that the total free energy of the system is at a minimum. In general, the minimal energy state will consist of a complex mixture of many compounds in low concentrations, and a small number of "major" compounds of relatively high concentration.

#### Standard Free Energy of Formation

Absolute values for the free energy function are rarely examined, but rather changes in free energy which occur when a given process takes place are considered. It is customary among chemists who work with isothermal systems to define, for each element at one atmosphere of pressure, an arbitrary standard state in either the solid, liquid, or diatomic gas phase. Then the standard free energy of formation of a compound,  $\Delta F_i^\circ$ , is defined as the difference in free energy between one mole of the compound at one atmosphere pressure and at a particular temperature and the total free energies of its elements in their standard states at the same temperature. These  $\Delta F_i^\circ$ 's are tabulated extensively in the chemical literature. In Table 40 we have compiled  $\Delta F_i^\circ$  values for 341 compounds, at four temperatures. It should be noted that the  $\Delta F_i^\circ$  value for the standard-state species of each element is zero at every temperature.

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\*See any general treatise on Chemical Thermodynamics.

In determining equilibrium concentrations in the ideal gas phase, it is sufficient to know the value of  $\Delta F_i^\circ$  and the atomic formula of each compound. Chemical reaction pathways are not specified in this method; equilibrium presumes only that at least one route exists leading to the production of each compound.

### Definition of Standard States

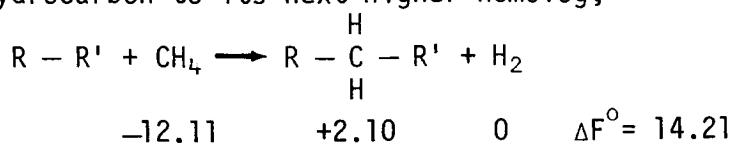
For carbon, the standard state which we have used in these calculations is graphite. For all other elements, the diatomic gases H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, P<sub>2</sub>, S<sub>2</sub> and Cl<sub>2</sub> have been used at all temperatures.

Several different phases are commonly in use for the standard states of sulfur and phosphorus. The Bureau of Mines Bulletin 595 uses the diatomic gas phase for sulfur throughout, while the JANAF tables refer to several standard-state phases, depending on the temperature: rhombic crystals, monoclinic crystals, liquid, and the ideal diatomic gas. The JANAF tables use solid red phosphorus and the diatomic gas as standard states for phosphorus, depending on the temperature. The computed distribution of compounds at equilibrium does not depend on the choice of standard compound, although the stated free energies of formation do. The use of more than one standard compound is inconvenient in making computations at many different temperatures. A discontinuity is introduced in the slope of the standard free energy versus temperature curve of every compound containing sulfur at each change of standard phase. It is troublesome to develop interpolation formulas for such discontinuous curves in order to generate free energies at intermediate temperatures. For convenience in computation, we have therefore chosen a single standard phase over the whole range of temperatures used. Where values have been obtained from the JANAF tables for sulfur and phosphorus compounds, they have been adjusted to be relative to the diatomic-gas standard states.

### Estimation of Free Energies from Group Contributions

For many organic compounds, the  $\Delta F_i^\circ$ 's have not been measured. However, it is often possible to estimate  $\Delta F_i^\circ$  for a compound from values measured for related compounds. The free energy of a compound can be expressed approximately as a sum of contributions from component radicals, shape factors, and the symmetry number. Van Krevelen and Chermin (1951) have worked out a set of group contribution values which fit a number of measured compounds with an average deviation of less than 0.5 kcal/mole. These values, interpolated for four temperatures, are shown in Table 41. Table 42 shows sample computations of the free energies of formation of three typical compounds, using group contributions.

The group contribution values may be used to ascertain the effect of substitutions, without specifying the exact structure of the parent compound. Thus, for the change from a hydrocarbon to its next higher homolog,



the equilibrium constant  $K_p$ , as derived below, is

$$K_p = \exp(-\Delta F/RT)$$

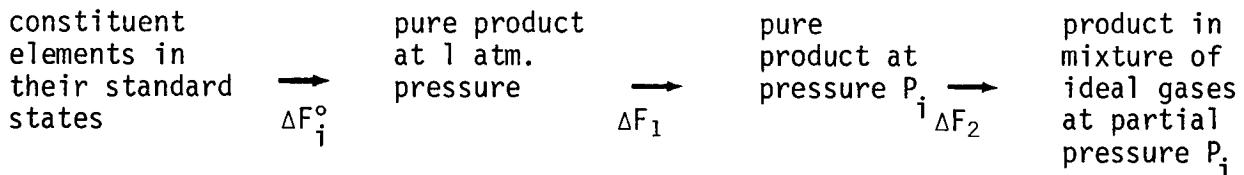
At 300° and 1 atm.,  $K_p = 5 \times 10^{-11}$ , or

$$\frac{[R-CH_2-R'] [H_2]}{[R-R'] [CH_4]} = 5 \times 10^{-11}$$

For regions where the partial pressures of  $H_2$  and  $CH_4$  are comparable, higher homologs will be much less stable than small compounds.

### Equilibrium Constants from Free Energies

In the ideal gas mixture, the free energy of a constituent at partial pressure  $P_i$ , relative to its component atoms in their standard states, can be determined from the following processes:



$\Delta F_i^\circ$  is the standard free energy of formation of the product at 1 atm. pressure from its constituent elements in their standard states. Such values are measured, or calculated routinely, by chemists, and tabulated in extensive compilations such as the JANAF Tables, American Petroleum Institute Research Project 44, U. S. Bureau of Mines Bulletins, National Bureau of Standards Circulars, etc. (see references, Table 40).

We calculate  $\Delta F_1$  from the definition for the free energy function:

$$F = E + PV - TS$$

or

$$dF = dE + PdV + VdP - TdS - SdT$$

For a reversible isothermal process

$$dT = 0$$

$$dE + PdV = TdS$$

For  $X$  moles of an ideal gas,

$$PV = XRT$$

Thus, for a reversible isothermal expansion from 1 atm. to pressure  $P_i$ ,

$$\int_1^{P_i} dF = \int_1^{P_i} VdP$$

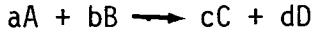
$$\Delta F_i = XRT \ln P_i$$

In this process  $\Delta F_2$  is zero, as the transfer of the compound may be made through a membrane permeable only to the compound, during which transfer there is no pressure change, so that  $\int VdP = 0$ . Summing the changes in free energies,  $\Delta F$ , during these processes, we find the free energy of 1 mole of gas at partial pressure  $P_i$  to be  $\Delta F_i = (\Delta F_i^\circ + RT \ln P_i)$ .

Thus, the free energy  $f_i$  of  $x_i$  moles of constituent  $i$  in the ideal gas mixture is given by

$$f_i = x_i [\Delta F_i^\circ + RT \ln P_i]$$

Suppose we have a system composed of four gases reacting according to the equation



When the concentrations of these four compounds are at equilibrium, the free energy change  $\Delta F$  in reacting an infinitesimal quantity of A and B to give C and D, is equal to zero.

$$\begin{aligned} \Delta F = -a [\Delta F_A^\circ + RT \ln P_A] - b [\Delta F_B^\circ + RT \ln P_B] + c [\Delta F_C^\circ + RT \ln P_C] \\ + d [\Delta F_D^\circ + RT \ln P_D] = 0 \end{aligned}$$

$$[-a \Delta F_A^\circ - b \Delta F_B^\circ + c \Delta F_C^\circ + d \Delta F_D^\circ] = -RT \ln [P_C^c P_D^d / P_A^a P_B^b]$$

The term on the left is the standard free energy change of the reaction,  $\Delta F^\circ$ . This quantity is derivable directly from the standard free energies of formation of the reactants and products. By definition we have

$$[P_C^c P_D^d / P_A^a P_B^b] = K_p$$

where  $K_p$  is the equilibrium constant in terms of the partial pressures of the gases. Thus we obtain the relationship which holds in general:

$$\Delta F^\circ = -RT \ln K_p \quad (1)$$

## Calculation of Chemical Equilibrium in Complex Mixtures

In our computer program the general method of White, Johnson, and Dantzig (1958) was followed for the determination of the balance of chemical species at equilibrium. The concentrations of the constituents are calculated which produce the minimum Gibbs free energy function for the mixture. This will represent the experimental equilibrium balance. With this method, no distinction in treatment is made among compounds. Each species to be included in the equilibrium is represented by one punched card on which are specified its name, molecular formula, and standard free energy of formation  $\Delta F_i^0$ . All possible equilibrium constants are simultaneously satisfied. The free energy  $F(X)$  of a mixture of  $n$  ideal gases containing  $X_i$  moles of the  $i^{th}$  chemical species is simply a sum of the total free energy contributions  $f_i$  of all species.

$$F(X) = \sum_{i=1}^n f_i = \sum_{i=1}^n X_i [ \Delta F_i^0 + RT \ln P + RT \ln (X_i / \bar{X}) ] \quad (2)$$

where  $P$  = the total pressure of the system

$T$  = the absolute temperature

$X_i$  = the number of moles of the  $i^{th}$  species

$$\bar{X} = \sum_{i=1}^n X_i, \text{ the total number of moles in the system} \quad (3)$$

$X = (X_1, X_2, X_3, \dots, X_n)$  the set of mole numbers

The determination of the equilibrium concentrations of the  $n$  chemical species is equivalent to determining the nonnegative set of values of  $X_i$  which minimizes the total free energy of the system and satisfies the mass-balance constraints for each element:

$$\sum_{i=1}^n A_{ij} X_i = B_j \quad j = 1, 2, \dots, m \quad (4)$$

where  $m$  = the number of elements

$A_{ij}$  = the number of atoms of species  $j$  per molecule of the  $i^{th}$  compound

$B_j$  = the total number of moles of atomic species  $j$  in the system

It will be shown below that the total free energy of the system is a concave function in the whole domain of positive concentrations. Therefore, in this region there is only one minimum and one corresponding set of positive mole fractions. We seek this set by an iterative procedure. For each computation, an initial combination of compounds consistent with the desired mass balance is stated. After each iterative step, the equilibrium set of concentrations is more nearly approximated, whatever the starting point.

To simplify the initial statement of concentrations, unstable "elements" with very large but arbitrary free energies may be introduced into the calculation. All of the mass is initially assigned to these elements. It rapidly distributes itself among more stable compounds during the calculation. A poor initial distribution is tolerated by the program; the necessary increase in computing time may be justified by the convenience.

We define

$$C_i = (\Delta F^\circ_i / RT) + \ln P$$

$$f_i = RT X_i [ C_i + \ln (X_i / \bar{X}) ], \quad \text{the total free energy contribution} \quad (5)$$

of the  $i^{\text{th}}$  compound.

For the purposes of computation we let  $X_i$  be an improved set of molecular concentrations which we may calculate from a prior estimate of the concentrations which we shall designate as  $Y_i$ .

In order to describe the iterative process, we need a mathematical expression for the improved molecular concentrations  $X_i$  in terms of the initial ones  $Y_i$ .

From equations (2) and (5), the free energy  $F(Y)$  of any system is

$$F(Y) = RT \sum_{i=1}^n Y_i [ C_i + \ln (Y_i / \bar{Y}) ] \quad (6)$$

where  $\bar{Y} = \sum_{i=1}^n Y_i$

Performing a Taylor-series expansion about the point  $Y$ , and letting

$$\Delta_i = X_i - Y_i$$

$$\bar{\Delta} = \bar{X} - \bar{Y}$$

we can obtain  $Q(X)$ , the quadratic approximation to  $F(X)$ :

$$Q(X) = F(Y) + \sum_i \frac{\partial F}{\partial X_i} \Big|_{X=Y} \Delta_i + (1/2) \sum_i \sum_k \frac{\partial^2 F}{\partial X_i \partial X_k} \Big|_{X=Y} \Delta_i \Delta_k \quad (7)$$

$$\frac{\partial F(X)}{\partial X_i} = RT [ C_i + \ln (X_i / \bar{X}) ] + 1 - \sum_i X_i / \bar{X} = RT [ C_i + \ln (X_i / \bar{X}) ]$$

$$\frac{\partial^2 F(X)}{\partial X_i^2} = RT [ (1/X_i) - (1/\bar{X}) ]$$

$$\frac{\partial^2 F(X)}{\partial X_i \partial X_k} = -RT/\bar{X} \quad \text{for } i \neq k$$

We note that  $Q(X)$  is always concave when all the  $X_i$ 's are positive. Then

$$Q(X) = F(Y) + RT \sum_i [c_i + \ln(Y_i/\bar{Y})] \Delta_i + (RT/2) \sum_i Y_i (\Delta_i/Y_i - \bar{\Delta}/\bar{Y})^2 \quad (8)$$

We use the method of steepest descents to find the next approximation to the mole fraction; so we must minimize  $Q(X)$ , subject to the constraint that the elemental composition remains fixed [see Eq (4)]. This is done by using the method of undetermined multipliers. We define  $Z(X)$  in terms of the multipliers  $\bar{F}_j$ :

$$Z(X) = Q(X) + \sum_{j=1}^m \bar{F}_j (- \sum_i A_{ij} X_i + B_j)$$

These multipliers will later be shown to be the partial molal free energies of the elements in the system.

Minimizing  $Z$ ,  $\frac{\partial Z}{\partial X_i} = 0$  for all  $i$ , we get the set of  $n$  equations for the  $n$  values of  $i$ .

$$\frac{\partial Z}{\partial X_i} = RT [c_i + \ln(Y_i/\bar{Y})] + RT (X_i/Y_i - \bar{X}/\bar{Y}) - \sum_{j=1}^m \bar{F}_j A_{ij} = 0 \quad (9)$$

Then

$$X_i = - (1/RT) f_i(Y) + \bar{X}(Y_i/\bar{Y}) + \left[ \sum_{j=1}^m (1/RT) \bar{F}_j A_{ij} \right] Y_i \quad (10)$$

where  $f_i(Y)$  is determined from the initial concentration  $Y_i$ , see Eq. (5). Summing over  $i$ , and multiplying by  $RT$ , we get, with the help of Eq. (4)

$$\sum_{j=1}^m \bar{F}_j B_j = \sum_{i=1}^n f_i(Y) = F(Y) \quad (11)$$

Substituting Eq. (10) in Eq. (4) gives  $m$  linear equations in the  $m+1$  unknowns  $\bar{F}_k$  and  $\bar{X}$ .

$$\sum_{k=1}^m R_{jk} (1/RT) \bar{F}_k / RT + B_j u = \sum_{i=1}^n (1/RT) A_{ij} f_i / RT \quad j = 1, 2, 3, \dots, m \quad (12)$$

$$\text{where } R_{jk} = \sum_{i=1}^n A_{ij} A_{ik} Y_i \quad \text{and } u = (\bar{X}/\bar{Y}) - 1$$

The  $m$  equations (12), along with Eq. (11), can now be solved for  $\bar{F}_j$  and  $u$ . From the solution, the new  $X_i$  values are found from Eq. (10). These now constitute an improved initial guess, as long as no  $X_i$  values are negative. If this should happen, a proportionally smaller step in each  $\Delta_i$  is taken to insure that all  $X_i$  be greater than 0. The free energy contributions  $f_i$  are now recomputed from Eq. (5), and the coefficients  $R_{jk}$  are recomputed from Eq. (12). New values for the  $\bar{F}_j$ 's and  $u$  are calculated from the linear equations (12). Using Eq. (10), an improved set of compound concentrations is calculated. This process is

continued until two successive distributions of species are as close together as desired. For this minimum solution,  $\bar{X} \approx \bar{Y}$  and  $X_i \approx Y_i$ . Equation (10) reduces to

$$f_i = Y_i \sum_{j=1}^m \bar{\mathfrak{F}}_j A_{ij} \quad (13)$$

### Calculation of Compound Concentrations from Tables of Partial Molal Free Energies

We are now able to derive the general equation relating compound concentrations to partial molal free energies. Substituting Eq. (13) in Eq. (5), we obtain the very important result:

$$x_i/\bar{X} = \exp \left[ \sum_{j=1}^m A_{ij} (\bar{\mathfrak{F}}_j/RT) - (\Delta F_i^\circ/RT) - \ln P \right] \quad (14)$$

The mole fraction concentrations of all constituents in a given system may be obtained from this key equation. In practice, the values of the partial molal free energies of the elements depend only on a few compounds which are present in significant concentration. Trace constituents do not contribute to the values of the  $\bar{\mathfrak{F}}_j$  and may be omitted from the solution. However, it is very important that all major constituents be included in order that the equilibrium be complete.

From Eq. (11) we see that the multipliers are simply the partial molal free energies of the elements:

$$\frac{\partial F(Y)}{\partial B_j} = \bar{\mathfrak{F}}_j$$

If we were to introduce into our mixture an infinitesimal number of moles of element j in its standard state (with free energy 0), the change in free energy of the system per mole of j would be  $\bar{\mathfrak{F}}_j$ , our undetermined multiplier.

The partial molal free energies  $\bar{\mathfrak{F}}_j$  of the j elements in a chemical system give a convenient characterization of the system. From them alone, the mole fraction concentration of any trace compound can be computed using Eq. (14).

Sample calculation of the concentration of any trace compound in any system. The standard free energy of formation and the molecular formula of the compound must be known. The partial molal free energies of the elements and the pressure and temperature of the system must be known. If the standard free energy of formation is not otherwise available, it can be estimated by the method of group contributions, as explained on page 170. The trace compound need not have been included in the computation of the partial molal free energies.

Let us calculate the mole fraction of acetic acid ( $C_2H_4O_2$ ) in the system C:H:O = 10:50:40 (Point A) at .2 atm. and 500°K. From Table 20a, we find the partial molal free energies of the elements in this system.

$$\bar{\mathfrak{F}}_C/RT = -0.689, \bar{\mathfrak{F}}_H/RT = -3.039, \text{ and } \bar{\mathfrak{F}}_O/RT = -48.632$$

From Table 40, compound number 100, we find the standard free energy of formation of acetic acid.

$$\Delta F_{\text{acet.ac.}}^{\circ} = -83.8 \text{ Kcal/mole}$$

substituting in Eq. (14), we get for the mole fraction of acetic acid:

$$\frac{x_{\text{acet.ac.}}}{x} = \exp \left\{ 2(-0.689) + 4(-3.039) + 2(-48.632) + \frac{83.8}{1.9864 \times 10^{-3} \times 500} + 1.609 \right\}$$
$$= 1.7 \times 10^{-11}$$

This answer may be compared with Table 20b, where the concentration for point A was also calculated by the computer as  $1.7 \times 10^{-11}$ . Similarly, the concentration of every compound in each system shown in Tables 1 to 39, part b, may be calculated from the  $\bar{\gamma}_j$  values for that system.

It is useful to tabulate some of these partial molal quantities to obtain some idea of their magnitudes in regions of various compositions. Table 43 shows a typical set of parameters for points in several regions. Physically, the added molecules of  $j$  would distribute themselves among the available compounds in the system. If a system at equilibrium contained free oxygen and oxygen was added, it would principally form  $O_2$  and  $\bar{\gamma}_O$  would be approximately half the  $\Delta F_j^{\circ}$  value for  $O_2$ , namely zero (except for pressure effects, which are small near 1 atm.). On the other hand, if we added  $H_2$ , the  $H_2$  would mainly form water;  $\bar{\gamma}_H$  would be roughly half the  $\Delta F_j^{\circ}$  for  $H_2O$ . Addition of C would lead to the formation of  $CO_2$  and the  $\bar{\gamma}_C$  would be determined mainly from  $\Delta F_j^{\circ}$  for  $CO_2$ . Similarly, a simple situation exists in systems containing excess hydrogen; but in the central reducing region, where a mixture of  $CH_4$ ,  $CO_2$ , and  $H_2O$  are all important the situation is more complex. In this region  $\bar{\gamma}_C$  is near zero.

#### Concentration Dependence of the Partial Molal Free Energies of the Elements

We have presented tables of partial molal free energies (in RT units) characterizing a great many systems (Tables 1 to 39, part a). From these, the concentration of any compound in any of the 45 systems can be calculated using Eq. (14). Values for systems of intermediate C, H, O elemental balances may be obtained by interpolation. In the first series (Tables 4-15, part a), where 80% nitrogen is added and the pressure is adjusted to 1 atm. in compensation, the values of  $\bar{\gamma}_j$  for C, H, and O are only slightly changed from those in a system of only C, H, and O at .2 atm. pressure.

The addition of trace amounts of the elements N, P, S, and Cl does not affect the  $\bar{\gamma}_j$  values of the major elements C, H, and O. It may be noted that in the second and third series of tables (16 to 39, part a), obtained by adding 0.01 or 0.0001 mole percent of N, P, S, and Cl to one total mole of C, H, and O, identical values for the partial molal free energies of C, H, and O are found. These values would be the same in a system containing only C, H, and O with no trace elements. The  $\bar{\gamma}_j$  values of the trace elements depend on their own concentrations and on the proportions of C, H, and O.

TABLE 43  
 PARTIAL MOLAL FREE ENERGIES,  $\bar{F}_j$ , AND PARTIAL PRESSURES,  $P_i$   
 Three Characteristic Systems at 1 atm. and 500°K

Composition	Partial molal free energies				Partial pressures			
	$\bar{F}_0$ /RT	$\bar{F}_H$ /RT	$\bar{F}_C$ /RT	$P_{O_2}$	$P_{H_2}$	$P_{CO_2}$	$P_{H_2O}$	$P_{CH_4}$
C : H : 0								
2 : 2 : 96	- .032	-28.289	-98.141	.94	.27x10 <sup>-24</sup>	.041	.021	0.
2 : 96 : 2	-55.773	-.045	-10.860	0.	.91	.13x10 <sup>-11</sup>	.043	.043
20 : 40 : 40	-48.418	-2.709	1.127	0.	.0044	.50	.33	.17
<hr/>								
Major Compounds				$\Delta F_i^\circ$ at 500°K				
O <sub>2</sub>				O <sub>2</sub>	0			
H <sub>2</sub>				H <sub>2</sub>	0			
CO <sub>2</sub>				CO <sub>2</sub>	-94.39			
H <sub>2</sub> O				H <sub>2</sub> O	-52.36			
CH <sub>4</sub>				CH <sub>4</sub>	-7.84			

We can derive the concentration dependence of  $\bar{\gamma}_j$  of trace element J from Eq. (14). This will permit us to calculate this  $\bar{\gamma}_j$  for systems different from those reported.

If there is only one important compound formed from trace element J, whose mole fraction is Z, we see from Eq. (14) that

$$\ln Z = \sum_{\substack{j=1, m \\ j \neq J}} A_{ij} (\bar{\gamma}_j / RT) - (\Delta F_i^0 / RT) + M (\bar{\gamma}_J / RT) - \ln P \quad (15)$$

where there are M atoms of the element J in this one important compound. For a different concentration of element J, in which this compound has a mole fraction  $Z'$ , the partial molal free energy of element J will change to  $\bar{\gamma}'_J$  while the free energies of the main elements in the system will remain unchanged. Substituting  $Z'$  and  $\bar{\gamma}'_J$  in Eq. (15) and subtracting the resulting equation from Eq. (15), we obtain:

$$\ln Z - \ln Z' = M \bar{\gamma}_J / RT - \bar{\gamma}'_J / RT$$

The partial molal free energy of J in this second system is:

$$\bar{\gamma}'_J / RT = (1/M) \ln (Z'/Z) + \bar{\gamma}_J / RT \quad (16)$$

$$\Delta \bar{\gamma}_J / RT = \ln (Z'/Z) \quad (17)$$

For trace elements which predominately form one compound,  $Z'/Z$  is just the ratio of the abundance of the trace element in the two systems.

Sample Calculation. As an example, let us calculate  $\bar{\gamma}_J$  in a system containing 0.0001% sulfur at the composition point C:H:O = 10:20:70. Let  $P = 20$  atm.,  $T = 500^\circ K$  (Table 21a). We know that  $H_2S$  is the only main compound containing sulfur in this system where  $S = 0.01\%$  and  $\bar{\gamma}_J / RT = -99.428$ . For our problem,

$$Z'/Z = 1/100, \quad \ln (Z'/Z) = -4.605$$

$$\text{Therefore, } \bar{\gamma}'_J / RT = -99.428 - 4.605 = -104.033$$

It may be readily confirmed that  $H_2S$  is the only main sulfur containing compound in the second system also. In Table 33a, the  $\bar{\gamma}_J$  value in the second system was actually calculated to be 104.043, within roundoff error of the above value.

Table 44 shows the corresponding change in  $\bar{\gamma}_J$  for the other trace elements in our system. A comparison of the values obtained in the computation of complete systems and calculated from Eq. (17) is shown.

If there is more than one main compound, as in the case of chlorine, the dependence of  $\bar{\gamma}$  on total concentration is more complex. There are two important chlorine containing compounds in the oxygen region,  $HCl$  and  $Cl_2$ . The partial molal free energies of chlorine and the concentration of each of its compounds also follows Eq. (16). However, since the concentrations are not equal to the known total chlorine concentrations, a more intricate computational scheme is needed to

TABLE 44  
DEPENDENCE OF PARTIAL MOLAL FREE ENERGIES OF TRACE CONSTITUENTS UPON ELEMENTAL CONCENTRATION  
System at 20 atm., 500 K, Tables 21a and 33a  
C:H:O = 10:20:70

	$\bar{\mathcal{F}}_C/RT$	$\bar{\mathcal{F}}_H/RT$	$\bar{\mathcal{F}}_0/RT$	$\bar{\mathcal{F}}_N/RT$	$\bar{\mathcal{F}}_P/RT$	$\bar{\mathcal{F}}_{C1}/RT$	$\bar{\mathcal{F}}_S/RT$	Mole Fractions
.01% N, P, S, Cl	-95.728	-26.130	1.151	-2.995	-163.602	-3.280	-99.428	Cl <sub>2</sub> HC1
.0001% N, P, S, Cl	-95.729	-26.130	1.151	-5.297	-164.754	-7.058	-104.043	3.7x10 <sup>-8</sup> 2.5x10 <sup>-6</sup>
$\Delta \bar{\mathcal{F}}/RT$					2.302	1.152	3.778	4.615
Important compounds				N <sub>2</sub>	P <sub>4</sub> O <sub>10</sub>	HC1, Cl <sub>2</sub>	S0 <sub>3</sub>	
M				2	4	--	--	1
$\bar{\mathcal{F}}_{M\Delta}/RT = \ln 100 = 4.605$ (Eq. (17))				4.604	4.608	--	--	4.615
$\ln [HC1]'/[HC1]$ (observed) = $\Delta \bar{\mathcal{F}}_{C1}/RT$						3.78		

obtain  $\bar{F}_{Cl}'$ . For example, an iterative process assuming initially that HCl is the only major chlorine containing compound might be followed. Using Eq. (16),  $\bar{F}_{Cl}'$  would be calculated. At each successive step, the concentrations of all the major chlorine containing constituents would be computed, and the available chlorine distributed proportionately. An improved  $\bar{F}'$  would then be calculated using Eq. (16).

Eq. (16) holds also for the case of systems containing 80% elemental nitrogen compared with those containing 0.01% elemental nitrogen. At a high nitrogen concentration, however, the partial pressure of N<sub>2</sub> is no longer proportional to the mole percentage.

### Errors Due to Uncertainties in Free Energy Values

The change in concentration of the *i*<sup>th</sup> minor constituent due to a change in  $\Delta F_i^\circ$  can be readily calculated from Eq. (14). If the difference between the first and second free energies is  $\delta_i$ , then the relation between the first concentration,  $X_1$ , and the second,  $X_2$ , is

$$X_2/X_1 = \exp(-\delta_i/RT)$$

Thus an increase in free energy of 1 kcal /mole at 300°K will lead to a decrease in concentration by a factor of 0.19. Table 45 shows a tabulation of typical values of the concentration ratios at various temperatures and the corresponding variations in free energies.

For many of the minor constituents, the free energies may sometimes be in error by one or two kcal / mole, particularly where these values are calculated from group contributions or quantum-mechanics principles.

TABLE 45  
CONCENTRATION CHANGE WITH CHANGE IN  $\Delta F^\circ$

Temperature	Concentration factor for a change in $\Delta F^\circ$ of 1 kcal.	Concentration factor for a change in $\Delta F^\circ$ of 0.1 kcal.
300°K	0.19	0.85
500°K	0.36	0.90
700°K	0.49	0.93
1000°K	0.60	0.95

The concentration of the trace constituents may also be affected by errors  $\epsilon_j$  in the partial molal free energies of the elements:

$$x_2/x_1 = \exp \left[ - \sum_{j=1}^m A_{ij} \epsilon_j \right]$$

These partial molal free energies of the elements  $\bar{F}_j$  are derived directly from the free energies of the major constituents, using at most small integral divisors. The  $\Delta F^\circ$  values for the major constituents are known to within 0.1 kcal/mole. The error introduced in the concentration of a trace compound would in general be less than that caused by 1.0 kcal/mole in Table 40.

The concentrations of the major compounds are generally fixed by the elemental composition of the system. Therefore they are not perceptibly influenced by small variations in the free energy values of these compounds.

### Metastable Systems

The applicability of our results to systems above the graphite phase boundary depends on the kinetic properties of these systems. At temperatures below 1000°K, solid graphite formation is often so slow that its rate is effectively zero. Before significant amounts of graphite could form, the smaller compounds in the system could effectively come to equilibrium. The larger aromatic compounds which build up sequentially from the small molecules (forming graphite in the limit) must be intermediate compounds. In our calculations we approximate this by assuming that rates are either infinite or zero, that is, each compound is either in the mixture or not. The validity of this approximation depends on the inclusion of the proper compounds in the system.

Compounds of four, five, or six rings are observed in plasma experiments and heat catalysed reactions. These compounds actually precipitate from the gas phase, and are not available for further reaction. (See Appendix II.)

We have approximated the effect of all aromatics higher than benzene and naphthalene by including one composite compound of 100 isomers of composition  $C_{22}H_{12}$ , which we call asphalt. The standard free energy  $\Delta F_i^\circ$  of one isomer is calculated by the method of group contributions. It may be shown that this composite is exactly equivalent to the 100 compounds if in all the computations we use the free energy  $\Delta F_c^\circ$ ,

$$\Delta F_c^\circ = \Delta F_i^\circ - RT \ln N$$

where  $N$  is the number of isomers, in this case 100.

The particular aromatics included in an equilibrium will affect the balance of compounds in regions where aromatics are major constituents. The concentrations of the aromatics themselves are influenced considerably while

the concentrations of nonaromatic compounds are rather independent of the exact nature of the aromatics included. In order to investigate the size of this effect, we present Tables 46 and 47 showing characteristics of systems of composition C:H:O = 30:30:40, well inside the asphalt region.

As we move up across the graphite line in the ternary diagram (see Fig. 1),  $\bar{\gamma}_C$  becomes positive in a system metastable with respect to graphite precipitation. The water concentration diminishes and  $\text{CO}_2$  and  $\text{CH}_4$  are formed as is shown in Table 46. The second column of this table shows values for a complete equilibrium while the third column shows the metastable system containing benzene, naphthalene, and asphalt but with graphite excluded.

TABLE 46

MOLE FRACTION OF MAJOR CONSTITUENTS IN THE SYSTEM  
C:H:O = 30:30:40 AT 500°K AND 1 ATM.

Compound	Mole Fraction of Main Constituents In Total System	
	Complete Equilibrium	Metastable System
$\text{CH}_4$	.02	.26
$\text{CO}_2$	.32	.73
$\text{H}_2\text{O}$	.30	$.94 \times 10^{-4}$
Benzene	$.22 \times 10^{-24}$	$.58 \times 10^{-4}$
Naphthalene	$<10^{-39}$	$.39 \times 10^{-4}$
Asphalt	$<10^{-39}$	$.47 \times 10^{-2}$
Graphite	.36	-----

The positive partial molal free energy of carbon leads to a gradual increase in the concentrations of organic compounds as carbon increases in the system. The major species are always  $\text{CH}_4$  and  $\text{CO}_2$ . At low temperatures, when the  $\text{CH}_4\text{-CO}_2$  line is crossed (the  $\text{CO-H}_2$  line at higher temperatures), the excess C must now appear in other compounds, the most stable of which are the polynuclear aromatics. The  $\bar{\gamma}_C$  rises further as this line is crossed. The asphalt threshold is mainly determined by the elemental composition of the system and the nature and identity of the carbon compounds, for example  $\text{CO}_2$ , CO, and  $\text{CH}_4$ , depending on conditions.

Table 47 shows the comparison of concentrations of selected compounds in systems containing varying combinations of aromatics. The bottom line shows the complete equilibrium for comparison. Here benzene is very dilute and polynuclear aromatics are  $<10^{-39}$  mole fraction. The top line shows the effect of omitting all aromatics. Ethane and other hydrocarbons are favored here. At low temperatures, as in the Fischer-Tropsch synthesis, aromatics are slow to form. This may then represent a metastable system in which petroleum would form by "equilibrium" processes.

TABLE 47  
EFFECT OF THE NUMBER OF AROMATIC COMPOUNDS IN THE EQUILIBRIUM ON THE PARTIAL MOLAL FREE ENERGIES AND COMPOUND CONCENTRATIONS  
C:H:O = 30:30:40 AT 500° K AND 1 ATM.

Aromatic Compounds Included in Equilibrium	Mole Fractions in Gas Phase						Benzene	Naphthalene	Anthracene	Asphalt
	$\frac{\partial G}{\partial C}/RT$	$\frac{\partial G}{\partial H}/RT$	$\frac{\partial G}{\partial O}/RT$	Acetylene	Ethane	Ethanol				
No aromatics	17.105	-6.598	-56.339	3.1x10 <sup>-12</sup>	9.5x10 <sup>-6</sup>	1.4x10 <sup>-3</sup>	4.4x10 <sup>-15</sup>	1.9x10 <sup>-10</sup>	1.3x10 <sup>-9</sup>	
Benzene	11.003	-5.076	-53.179	3.2x10 <sup>-16</sup>	2.1x10 <sup>-8</sup>	6.6x10 <sup>-5</sup>	4.8x10 <sup>-15</sup>	1.0x10 <sup>-11</sup>	1.6x10 <sup>-9</sup>	1.9x10 <sup>-2</sup>
Benzene and Naphthalene	10.395	-4.917	-52.873	1.3x10 <sup>-16</sup>	1.2x10 <sup>-8</sup>	5.1x10 <sup>-5</sup>	5.1x10 <sup>-15</sup>	7.6x10 <sup>-12</sup>	1.6x10 <sup>-9</sup>	1.3x10 <sup>-3</sup>
Benzene, Naphthalene and Anthracene	10.305	-4.892	-52.828	1.2x10 <sup>-16</sup>	1.1x10 <sup>-8</sup>	4.9x10 <sup>-5</sup>	5.1x10 <sup>-15</sup>	7.3x10 <sup>-12</sup>	1.6x10 <sup>-9</sup>	8.8x10 <sup>-4</sup>
Benzene, Naphthalene and Asphalt*	9.691	-4.733	-52.521	4.7x10 <sup>-17</sup>	6.0x10 <sup>-9</sup>	3.7x10 <sup>-5</sup>	5.3x10 <sup>-15</sup>	5.5x10 <sup>-12</sup>	1.7x10 <sup>-9</sup>	5.8x10 <sup>-5</sup>
Benzene, Naphthalene and Asphalt†	9.691	-4.733	-52.521	4.7x10 <sup>-17</sup>	6.0x10 <sup>-9</sup>	3.7x10 <sup>-5</sup>	5.3x10 <sup>-15</sup>	5.0x10 <sup>-12</sup>	1.7x10 <sup>-9</sup>	3.9x10 <sup>-5</sup>
Graphite included along with all aromatics	0	-2.802	-47.873	8.4x10 <sup>-24</sup>	5.2x10 <sup>-14</sup>	1.5x10 <sup>-8</sup>	2.3x10 <sup>-16</sup>	5.0x10 <sup>-15</sup>	1.6x10 <sup>-10</sup>	3.5x10 <sup>-24</sup>
									0.	0.

\* (100 isomers of  $C_{22}H_{12}$ )

For the other combinations of aromatics included, the composite of all isomers of the largest polynuclear aromatic is the most concentrated aromatic. Adding anthracene to a system which already contains benzene, naphthalene, and asphalt makes an imperceptible difference. It can be seen that the order of magnitude of the nonaromatic compounds is independent of the particular species of aromatics included.

### References

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## **Chapter 3**

### **Program Chem-Equilibrium**

## PROGRAM CHEM-EQUILIBRIUM

## Program Description

Program CHEM-EQUILIBRIUM calculates the balance at thermodynamic equilibrium of chemical species present in an ideal gas mixture of specified elemental composition. An explanation of the method is given in Chapter 2, following that described by White, Johnson and Dantzig (1958)\*. At specified pressure and temperature, the concentration balance follows directly from the identities of the compounds considered present, their standard free energies of formation, and their molecular formulas. The equilibrium state is that particular distribution of molecular composition  $X_i$ , which produces a minimum total free energy for the system while maintaining the elemental composition unchanged.

An iterative method of solution is followed. Compounds which are expected to be important, called major components, are treated separately. Using rough initial guesses of the concentrations of these compounds, which incidentally define the elemental composition, an improved approximation to the compound concentrations is determined. This step involves the solution of  $(M + 1)$  linear equations, where  $M$  is the number of elements present. These new concentrations are then used as the initial guesses for the next stage of the approximation. When, in two successive iterations, for all compounds and elements,

$$\frac{\text{Change in } X_i}{X_i} \leq CP \text{ and}$$

$$\frac{\text{Change in } \mathfrak{F}_j}{\mathfrak{F}_j} \leq CP$$

the problem is terminated. If these conditions are not met after a given number of iterations, ITNUM, the problem is deleted. Both CP and ITNUM are read in as initial data. Since the program never improves a zero concentration, a small minimum initial value, CSTART, is given to all major components not otherwise assigned a concentration. Since this produces a very slight change in the elemental composition of the system, a suitably small number must be chosen for CSTART.

During the iterative procedure, no compound concentration can be negative. If this is indicated, the increments of concentration are scaled down so that all concentrations remain positive. In order to prevent large oscillations during the first few iterations, provision is made for further scaling.

\*White, W. B., Johnson, S. M. and Dantzig, G. B., J. Chem. Phys., 28, 751 (1958).

If the concentration of any compound becomes very small during an iteration, convergence is hindered. Compounds are therefore removed from the list of major components if their concentrations fall below a given CONCMN, also an input parameter, and placed with the trace components. However, the linear equations cannot be solved if there are fewer major components than elements, and therefore at least this minimum number of major components is always maintained. When the computation is completed, a check is made to see whether any trace compound has a concentration greater than TRACMX, another input parameter. If there are none, the solution is correct. If any do exist, the offending trace constituents are placed with the major components and given the initial concentration of CSTART, and the problem is solved again. The program almost always converges to a solution, even where a very poor initial guess has been made. The statement of elemental composition is particularly easy for "monoatomic" compounds. Such convenient fictitious compounds, assigned arbitrary high free energy values, may be included and may constitute all of the initial elemental composition. Convergence is usual, although the program operates more slowly with such a poor guess.

A large number of equilibrium systems may be considered in one computer run, provided the compounds present are the same for all systems. Pressure, temperature and elemental compositions may vary in one computer run. For each specified pressure and temperature, systems with many different elemental compositions may be considered. The equilibrium concentrations for each of these systems may optionally be printed out immediately. The results are also stored, and ternary diagrams produced summarizing values at all elemental compositions. The ternary diagrams produced show the concentration of each compound and the value of the partial molal free energy of each element for all elemental compositions considered. In addition, tables of concentrations of all compounds at nine selected elemental compositions, and of partial molal free energies at all composition points, may be obtained. Alternatively, initial guess cards may be punched from the solutions. Any number of pressure and temperature conditions may be specified in a single run.

Portions of ternary diagrams may be enlarged by specifying TX, a magnification factor. The origin is automatically located from the composition points supplied. Values may be plotted to the edge of the computer print-out paper.

. For any run, as many as 100 compounds can be considered. The systems may contain up to 15 elements. Seventy systems of varying elemental composition can be considered, but there is an additional constraint, imposed by the total storage available:

$$(NC + NE + 3) \cdot (EC) \leq 4000$$

where

NC = number of compounds

NE = number of elements

EC = number of systems with  
different elemental compositions

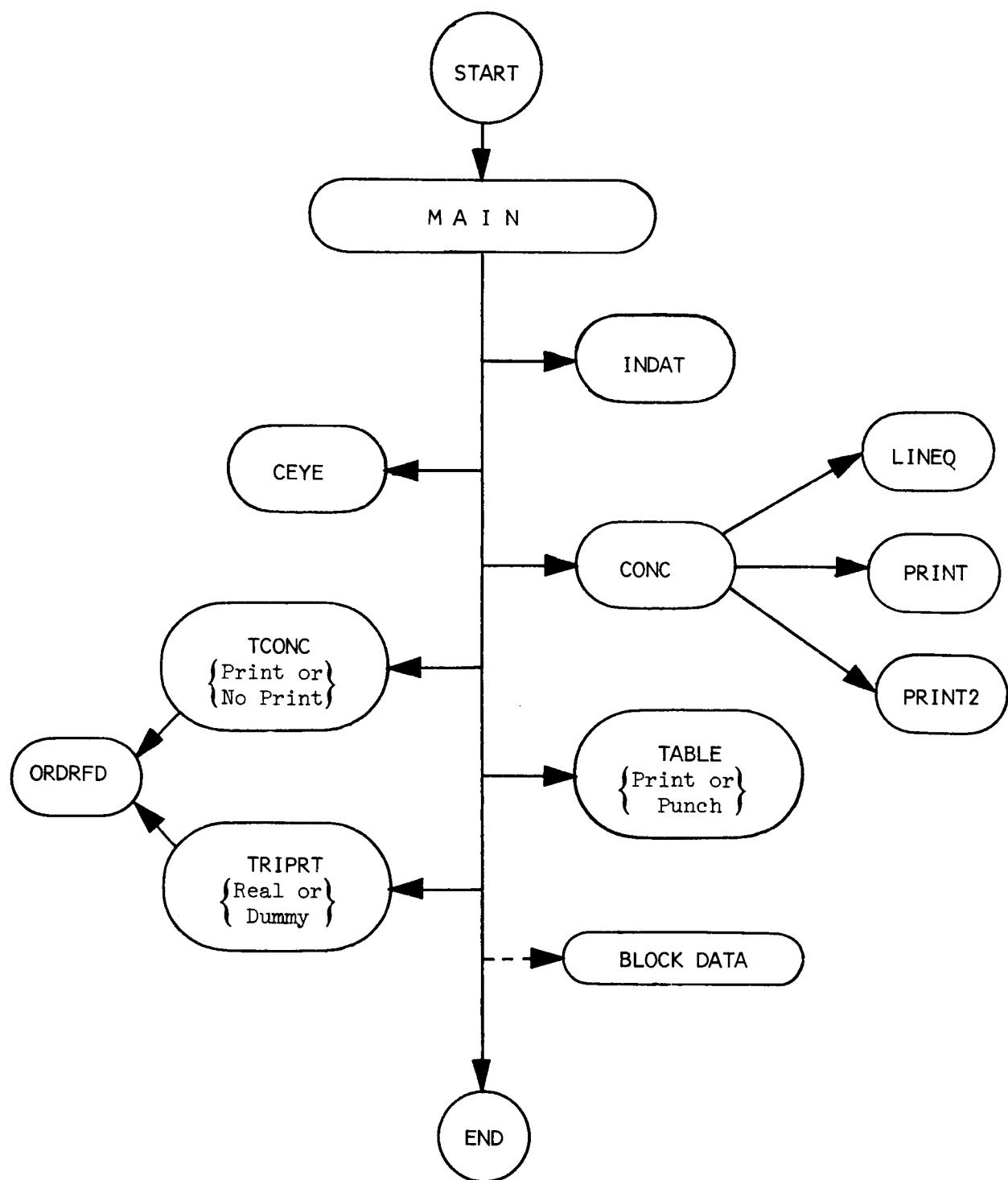
## Subprogram Listing

### SUBPROGRAMS

MAIN	Reads title, constants, initial guesses, numbers of selected runs, pressure and temperature.
INDAT	Reads temperatures of free energy table, names of chemical species, their free energies, formulae and tag.
CEYE	Approximates free energies of chemical species for a current temperature using a parabolic approximation.
CONC	Computes partial molal free energies of elements and concentrations of major compounds in mass balance.
LINEQ	Solves a system of linear equations.
PRINT	Dummy routine, providing entry to convergence process of CONC routine.
PRINT2	Prints out total free energy of system and number of iterations made.
TCONC	(Print) Computes concentrations of all compounds, stores necessary items for a print out of triangular diagrams and prints out elemental free energies and concentrations of compounds. (No print) Computes concentrations of all compounds, stores necessary items for a print out of triangular diagrams.
ORDRFD	Arranges a list of numbers in a descending order and reorders an associated list.
TABLE	(Print) Prints out a table of elemental free energies and a table of compound concentrations for up to nine elemental compositions. (Punch) Punches out initial guess cards from the solutions found.
TRIPRT	Prints out triangular diagrams for each $\bar{F}$ and each compound concentration. Prints complete grid diagram or a magnified portion of a diagram. A dummy program may replace TRIPRT in case diagrams are not desired.
BKDT	Statement to provide a table of names of elements.

Program CHEM-EQUILIBRIUM

SUBPROGRAM LINKAGE



# PROGRAM CHEM-EQUILIBRIUM

## Data Card Order and Formats

### A. Order of Data Cards:

- (1) Title card (1 card)
- (2) Constant card (1 card)
- (3)  $\Delta F^\circ$  Temperature card (1 card)
- (4) Chemical species data cards (major - arbitrary number of cards)  
End of major compounds card (1 card)  
  
Chemical species cards (trace - arbitrary number of cards)  
End of trace compounds card (1 card)
- (5) Initial concentration cards (arbitrary number of sets of  
NGUESS/2 cards)  
End cards (NGUESS/2 blank cards)
- (6) NUMRUN card (1 card)
- (7) Pressure and temperature cards (arbitrary number of cards)  
Systems with the elemental compositions specified in (5) above  
are calculated and plotted for each set of external conditions,  
P and T.

### B. Data Cards Formats:

#### (1) Title card

Field 1 - 72 TITLE (I) Format 12A6

#### (2) Constant card

Field 1 - 10 CSTART F 10.9 minimum concentration allowed  
for a major constituent ( $10^{-5}$   
if blank)

11 - 20 TRACMX F 10.9 maximum concentration permitted  
for a trace constituent ( $3 \times 10^{-4}$  if blank)

21 - 30 CONCMN F 10.9 compounds are made minor if  
their concentrations become less  
than CONCMN ( $10^{-5}$  if blank)

31 - 40	ITNUM	I 10	problem is deleted if more than maximum number of ITNUM iterations are needed (30 if blank)
41 - 50	NGUESS	I 10	maximum number of major compounds whose initial concentrations are specified (20 if blank)
51 - 60	CP	F 10.9	convergence parameter; maximum relative change in concentrations between two iterations ( $10^{-3}$ if blank)
61 - 70	TX	F 10.0	scale factor for ternary diagrams (1.0 if blank)

(3) Three Temperatures Card:

Field 1 - 10	TT (1)	F 10.5	$\Delta F^\circ$ values are given at these three temperatures for each compound in the system. Parabolic interpolation or extrapolation is made for other temperatures.
11 - 20	TT (2)	F 10.5	
21 - 30	TT (3)	F 10.5	

(4) Chemical Species, Free Energy, Molecular Formula:

Constituent cards are all punched as follows:

Field 1 - 15	CHEM (I, J)	3A6	compound names of up to 15 characters should start in column 1
19 - 25	DF (I, 1)	F 7.3	free energies of formation at the three temperatures specified on temperature card (3).
26 - 32	DF (I, 2)	F 7.3	
33 - 39	DF (I, 3)	F 7.3	
40 - 41	XNA (1)	A 2	element name, the right column should be used for a single letter
42 - 43	NF (1)	I 2	molecular formula, right adjust numbers e.g., 40 41 42 43 44 45 46 47 C 1 0 2 H 1 C L 1

•      •      •  
•      •      •  
•      •      •  
64 - 65 XNA (7) A 2

66 - 67 NF (7) I 2

72       TAG       A 1       TAG character is printed preceding the compound name where free energies are listed

Major constituents come first, followed by an end card:

Field 42 - 43 00  
46 - 47 11

Minor constituents come next, followed by a second end card:

Field 42 - 43 00  
46 - 47 00

(5) Initial Concentrations of Compounds:

Each set of NGUESS/2 cards defines the elemental composition for one system. Any number of systems may be specified up to 70.

Field 1 - 15 STR (1, J) 3A6	Compound name
19 - 28 GF (1) F 10.8	Total number of moles in system
29 - 43 STR (2, J) 3A6	Compound name
47 - 56 GF (2) F 10.8	Total number of moles in system

All major compounds are automatically assigned a concentration of at least CONCMN, specified on the constant card (2). STR (1, 1) should not be blank.

A set of NGUESS/2 blank cards must follow the specified systems to indicate the end of the initial concentration cards: {If NGUESS is odd, then (NGUESS + 1)/2 cards are needed.}

(6) NUMRUN Card:

Format 9I4

A table of compound concentrations from up to nine specified runs is formed. The numbers correspond to the set of initial concentrations in (5).

(7) Pressure and Temperature Card:

Field	1 - 10	PP	F 10.5	pressure in atmospheres
	11 - 20	T	F 10.5	temperature in °K

Any number of pressure and temperature conditions may be specified. For each condition, systems of all elemental compositions specified in (5) will be calculated.

STANDARD DISCLAIMER FOR COMPUTER PROGRAMS

Although each program has been tested by the author, no warranty, express or implied, is made by the author, nor shall the fact of distribution constitute any such warranty, and no responsibility to others is assumed by the authors.

Program CHEM-EQUILIBRIUM

Listing of Fortran IV Statements

```

C MAIN PROGRAM OF CHEM-EQ SYSTEM
C READS TITLE, CONSTANTS, INITIAL GUESSES, NUMBERS OF SELECTED RUNS,
C PRESSURE AND TEMPERATURE.
C CALLS SUBROUTINES INDAT, CEYE, CONC, TCONC, TABLE AND TRIPRT.
C
COMMON /ELK1/XNA(15),XNAM(15),R(17,17),P(16),BAL(15),NUM(16),B(15)
COMMON /BLK2/TITLE(12),GF(20),TT(3),XX(15),AF(50),AELE(50),
1ELEMTS(15)
COMMON /BLK3/X(100),Y(100),A(100,15),C(100),SF(100),CHEM(100,3),
1DF(100,3),DEL(100),STR(100,3),STR2(100,3),XK(100),CNC(100)
COMMON /BLK5/CPRT(4000)
COMMON /BLK6/MAJOR(100),ITRACE(100)
COMMON /BLK7/M,NMAJOR,NTRACE,NN,XB,YB,T,PP,LAMDA,CP,ITNUM,TRACMX,
1CONCMN,CSTART,NRUNS,LINE,LAST,KIP,NPP,ITP,IOT,TX,CURPLT
COMMON /BLK9/NR
COMMON /BLK10/NUMRUN(9)
DIMENSION NA(15)*NAM(15),NF(20),ICH(100,3),IDEL(100),ISTR(100,3),
1ISTR2(100,3),IXX(15)
DIMENSION NSAVE(70,20),GESAVE(70,20)
DIMENSION NCPRT(4000)
EQUIVALENCE (XNA(1),NA(1)),(XNAM(1),NAM(1)),(GF(1),NF(1)),
1(CHEM(1),ICH(1)),(DEL(1),IDEL(1)),(STR(1),ISTR(1)),(STR2(1),ISTR2(
21)),(CURPLT,NURPLT),(BL,IBL),(XX(1),IXX(1))
EQUIVALENCE (CPRT(1),NCPRT(1))
DOUBLE PRECISION R,P,BAL,B,X,Y,A,C,SF,DEL,XB,YB,LAMDA
DATA BL/0606060606060/
C SPECIFY INPUT AND OUTPUT TAPE UNITS. INITIALIZE NRUNS AND MAXKNT
ITP=5
IOT=6
NRUNS=0
MAXKNT=5
C FOLLOWING STATEMENTS (THROUGH 1) ARE INTRODUCED SIMPLY TO AVOID
C PRINT OUT OF UNDERFLOW MESSAGES WITHIN FINAL RESULTS
      WRITE(IOT,1000)
1000 FORMAT(1H15X,67H THE FOLLOWING MESSAGES ON THIS PAGE ARE NOT A PAR
1T OF THE RESULTS./1H05X,27H PLEASE TEAR OFF THIS PAGE.)
      DO 1 I=1,6
      SMALL=1.E-37
      TIME=0.5
      1 PRODCT=SMALL*TIME
C READ TITLE. CALL SUBROUTINE INDAT AND WRITE CONSTANTS
READ(ITP,200) (TITLE(I),I=1,12)
READ(ITP,201) CSTART,TRACMX,CONCMN,ITNUM,NGUESS,CP,TX
IF(CSTART.EQ.0.0) CSTART=0.00001
IF(TRACMX.EQ.0.0) TRACMX=0.0003
IF(CONCMN.EQ.0.0) CONCMN=0.00001
IF(ITNUM.EQ.0) ITNUM=30
IF(NGUESS.EQ.0) NGUESS=20
IF(CP.EQ.0.0) CP=0.001
IF(TX.EQ.0.0) TX=1.0
      WRITE(IOT,202) (TITLE(I),I=1,12)
      WRITE(IOT,203) (TITLE(I),I=1,12)
      CALL INDAT
      WRITE(IOT,204) CSTART,TRACMX,CONCMN,CP,ITNUM,NGUESS,TX
C READ INITIAL GUESSES FOR NRUNS. SAVE SERIAL NUMBERS OF GUESS
C COMPOUNDS AND THEIR CONCENTRATIONS
      5 NRUNS=NRUNS+1
      READ(ITP,205) ((STR(I,J),J=1,3),GF(I),I=1,NGUESS)
      IF(ISTR(1,1).EQ.IBL.AND.ISTR(1,2).EQ.IBL.AND.ISTR(1,3).EQ.IBL) GO
1TO 25
      DO 20 J=1,NGUESS
      DO 10 I=1,NMAJOR
      IF(ISTR(J,1).EQ.ICH(I,1).AND.ISTR(J,2).EQ.ICH(I,2).AND.ISTR(J,3).E
1Q.ICH(I,3)) GO TO 15
      10 CONTINUE
      GESAVE(NRUNS,J)=0.0

```

```

      IF(ISTR(J,1).EQ.IBL.AND.ISTR(J,2).EQ.IBL.AND.ISTR(J,3).EQ.IBL) GO
1 TO 20
      WRITE(IOT,212) (STR(J,JJ),JJ=1,3),GF(J),NRUNS
      GO TO 20
15 NSAVE(NRUNS,J)=MAJOR(I)
      GESAVE(NRUNS,J)=GF(J)
20 CONTINUE
      GO TO 5
25 NRUNS=NRUNS-1
C READ NUMBERS OF SELECTED RUNS FOR A PRINT OUT OF SUMMARY TABLE
      READ(ITP,211) (NUMRUN(I),I=1,9)
C READ PRESSURE AND TEMPERATURE OF CURRENT SYSTEM
C (IF PP AND T ARE BOTH ZERO -I.E., A BLANK CARD - JOB TERMINATES)
      N24=-1
30 READ(ITP,206) PP,T
      N24=N24+1
      IF(PP.EQ.0.0.AND.T.EQ.0.0) GO TO 100
C INITIALIZE PAGE NUMBER AND NR. CALL SUBROUTINE CEYE AND INITIALIZE
C CPRT
      NPP=0
      NR=0
      CALL CEYE
      IH=(M+NN+3)*NRUNS
      DO 31 I=1,IH
      31 CPRT(I)=0.0
C
C FROM HERE THROUGH STATEMENT 90 WILL BE REPEATED UNTIL NR=NRUNS FOR
C EACH SYSTEM
C
C REINITIALIZE KOUNT, NMAJOR, NTRACE AND SERIAL NUMBERS OF MAJOR AND
C TRACE COMPOUNDS
      35 KOUNT=0
      NR=NR+1
      NMAJOR=NORMAJ
      NTRACE=NN-NMAJOR
      DO 45 I=1,NN
      IF(I.GT.NMAJOR) GO TO 40
      MAJOR(I)=I
      GO TO 45
      40 ISUB=I-NMAJOR
      ITRACE(ISUB)=I
      45 CONTINUE
C INITIALIZE CONCENTRATIONS OF MAJOR COMPOUNDS TO CSTART AND THOSE OF
C TRACE COMPOUNDS TO ZERO
      DO 36 I=1,NMAJOR
      36 Y(I)=CSTART
      IL=NMAJOR+1
      DO 37 I=IL,NN
      37 Y(I)=0.0
      IF(N24.GT.0) GO TO 50
      NPP=NPP+1
      WRITE(IOT,207) (TITLE(I),I=1,12),NPP
C REPLACE CONCENTRATIONS OF GUESS COMPOUNDS WITH THOSE READ IN AND
C WRITE OUT
      50 DO 55 I=1,NGUESS
      IF(GESAVE(NR,I).EQ.0.0) GO TO 55
      IND=NSAVE(NR,I)
      Y(IND)=GESAVE(NR,I)
      IF (N24.GT.0) GO TO 55
      WRITE(IOT,208) (CHEM(IND,J),J=1,3),Y(IND)
      55 CONTINUE
C INITIALIZE LINE. COMPUTE YB AND CALL SUBROUTINE CONC
      60 YB=0
      LINE=0
      DO 65 J=1,NMAJOR
      IND=MAJOR(J)
      65 YB=YB+Y(IND)
      70 CALL CONC
C IF LINE IS 1 (NO SOLUTIONS WITHIN ITNUM ITERATIONS), PROCEED TO NEXT
C RUN. OTHERWISE CALL SUBROUTINE TCONC
      IF(LINE.EQ.1) GO TO 90
      75 CALL TCONC

```

```

C IF LINE IS ZERO PROCEED TO NEXT RUN. IF NOT (SOME COMPOUNDS MOVED
C FROM TRACE TO MAJOR OR VICE VERSA), CHECK WHETHER MAXKNT TRIALS HAVE
C BEEN CARRIED OUT. IF SO, WRITE INFORMATION AND PROCEED TO NEXT RUN.
C OTHERWISE REDO WITH CURRENT VALUES.
    IF(LINE.NE.1) GO TO 90
    80 WRITE(IOT,210)
    KOUNT=KOUNT+1
    IF(KOUNT.GT.MAXKNT) GO TO 85
    GO TO 60
    85 WRITE(IOT,209) MAXKNT
    90 IF(NR.LT.NRUNS) GO TO 35
C END OF COMPUTATIONS FOR CURRENT SYSTEM
C
C CALL SUBROUTINES TABLE AND TRIPRT
    CALL TABLE
    CALL TRIPRT
C GO BACK TO READ NEXT SET OF PP AND T FOR NEXT SYSTEM
    GO TO 30
C
C FORMAT SPECIFICATIONS
C
    200 FORMAT(12A6)
    201 FORMAT(3F10.9,2I10,F10.9,F10.0)
    202 FORMAT(1H1/1H210X,12A6)
    203 FORMAT(1H110X,12A6)
    204 FORMAT(1H05X,8H REMARKS//6X,33H INITIALIZE ZERO CONCENTRATION TO E
        110.2/6X,31H REDO IF TRACE COMPOUNDS EXCEED E11.3/7X,58HREDO IF CON
        2CENTRATIONS OF MAJOR COMPOUNDS BECOME LESS THAN E11.3/6X,73H ITERA
        3TION TERMINATES WHEN ALL CONCENTRATIONS AND ELEMENTAL FREE ENERGIE
        4S/8X,42H ON TWO SUCCESSIVE ITERATIONS AGREE WITHIN E10.3,14H * 100
        5 PERCENT/6X,45H MAXIMUM NUMBER OF ITERATIONS TO BE TRIED IS I2/6X,
        665H NUMBER OF COMPOUNDS WHOSE INITIAL CONCENTRATIONS ARE GUESSED I
        7S I2/6X,48H TRIANGLE PRINT OUT IS MAGNIFIED BY A FACTOR OF F6.1)
    205 FORMAT(2(3A6,F10.8))
    206 FORMAT(2F10.5)
    207 FORMAT(1H110X,12A6,10X,5H PAGEI4/1H08X,5H NAME,7X,6H PHASE,7X,14H
        1INITIAL GUESS//)
    208 FORMAT(7X,3A6,10X,F10.5)
    209 FORMAT(1H05X,71H THE SYSTEM WITH THIS INITIAL GUESS HAS NOT REACHE
        1D STEADY STATE AFTER I2,11H ITERATIONS/6X,25H GO TO NEXT INITIAL G
        2UESS)
    210 FORMAT(1H05X,48H SOME COMPOUNDS MOVED FROM OR TO TRACE COMPONENT)
    211 FORMAT(9I4)
    212 FORMAT(1H07X,25H NOTE ... GUESS COMPOUND 3A6,20H WITH CONCENTRATIO
        1N F10.8,15H IN RUN NUMBER I2,24H IS NOT A MAJOR COMPOUND/17X,29H T
        2HIS COMPOUND IS ELIMINATED.)
100 STOP
END

```

```

C SURROUNGE INDAT OF CHEM-EQ SYSTEM
C READS TEMPERATURES OF FREE ENERGY TABLE, NAMES OF CHEMICAL SPECIES,
C THEIR FREE ENERGIES, FORMULAE AND TAG.
C
SUBROUTINE INDAT
COMMON /BLK1/XNA(15),XNAM(15),R(17,17),P(16),BAL(15),NUM(16),B(15)
COMMON /BLK2/TITLE(12),GF(20),TT(3),XX(15),AF(50),AELE(50),
1ELFMTS(15)
COMMON /BLK3/X(100),Y(100),A(100,15),C(100),SF(100),CHEM(100,3),
1DF(100,3),DEL(100),STR(100,3),STR2(100,3),XK(100),CNC(100)
COMMON /BLK6/MAJOR(100),ITRACE(100)
COMMON /BLK7/M,NMAJOR,NTRACE,NN,XB,YB,T,PP,LAMDA,CP,ITNUM,TRACMX,
1CONCMN,CSTART,NORMAJ,NRUNS,LINE,LAST,KIP,NPP,ITP,IOT,TX,CURPLT
DIMENSION NA(15),NAM(15),NF(20),ICH(100,3),IDEL(100),ISTR(100,3),
1ISTR2(100,3),IXX(15)
EQUIVALENCE (XNA(1),NA(1)),(XNAM(1),NAM(1)),(GF(1),NF(1)),
1(CHEM(1),ICH(1)),(DEL(1),IDEL(1)),(STR(1),ISTR(1)),(STR2(1),ISTR2(
21)),(CURPLT,NURPLT),(BL,IBL),(XX(1),IXX(1))
DOUBLE PRECISION R,P,BAL,B,X,Y,A,C,SF,DEL,XB,YB,LAMDA
DATA BLANKS/060606060606/

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```

C INITIALIZE M, NN, NMAJOR, NTRACE, XNAM(I), AND A(I,J)
M=0
NN=0
NMAJOR=0
NTRACE=0
BL=BLANKS
DO 1 I=1,15
XNAM(I)=0.0
DO 1 J=1,100
1 A(J,I)=0.0
INDEX=1
C READ AND WRITE OUT THREE TEMPERATURES OF FREE ENERGY TABLE
READ(ITP,101) (TT(I),I=1,3)
WRITE(IOT,102) (TT(I),I=1,3)
C READ CHEMICAL SPECIES CARDS (NAME, FREE ENERGIES, FORMULA AND TAG)
C END OF MAJOR COMPOUND IS INDICATED BY A CARD WITH NF(1)=00 AND
C NF(2)=11
C END OF TRACE COMPOUND IS INDICATED BY A CARD WITH NF(1)=00 AND
C NF(2)=00
5 NN=NN+1
READ(ITP,103) (CHEM(NN,J),J=1,3),(DF(NN,J),J=1,3),(XNA(J),NF(J),
1J=1,7),TAG
IF(NF(1)) 20,10,20
10 NN=NN-1
IF(NF(2)) 15,75,15
15 NMAJOR=NN
NORMAJ=NMAJOR
WRITE(IOT,104)
INDEX=2
GO TO 5
20 GO TO (25,70),INDEX
C STORE SERIAL NUMBER OF MAJOR COMPOUND IN MAJOR(I)
25 MAJOR(NN)=NN
C STORE NAME OF NEW ELEMENT IN XNAM(I) AND NUMBERS OF ELEMENTS OF A
C COMPOUND IN A(I,J)
30 DO 60 J=1,7
IF(NA(J)-IBL) 35,65,35
35 IF(M) 40,50,40
40 DO 45 JK=1,M
IF(NA(J)-NAM(JK)) 45,55,45
45 CONTINUE
50 M=M+1
XNAM(M)=XNA(J)
JK=M
55 A(NN,JK)=NF(J)
60 CONTINUE
JL=7
65 JL=J-1
C WRITE OUT CHEMICAL SPECIES (TAG, NAME, FREE ENERGIES, AND FORMULA)
WRITE(IOT,105) TAG,(CHEM(NN,J),J=1,3),(DF(NN,J),J=1,3),(XNA(J),
1NF(J),J=1,JL)
GO TO 5
C STORE SERIAL NUMBER OF TRACE COMPOUND IN ITRACE(I)
70 NTRACE=NN-NMAJOR
ITRACE(NTRACE)=NN
GO TO 30
75 RETURN
C
C FORMAT SPECIFICATIONS
C
101 FORMAT(3F10.5)
102 FORMAT(1H011X,5H NAME,7X,6H PHASE,7X,32H FREE ENERGY(DF) AT TEMPER
1ATURES,7X,8H FORMULA/34X,3F11.2/1H05X,17H MAJOR COMPONENTS//)
103 FORMAT(3A6,3F7.3,7(A2,I2),4X,A1)
104 FORMAT(1H05X,17H TRACE COMPONENTS//)
105 FORMAT(8X,A1,1X,3A6,7X,3F11.3,8X,10(A2,I2))
END

```

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C SUBROUTINE CEYE OF CHEM-EQ SYSTEM
C APPROXIMATES FREE ENERGIES OF CHEMICAL SPECIES FOR A CURRENT
C TEMPERATURE
C
SUBROUTINE CEYE
COMMON /BLK1/XNA(15),XNAM(15),R(17,17),P(16),BAL(15),NUM(16),B(15)
COMMON /BLK2/TITLE(12),GF(20),TT(3),XX(15),AF(50),AELE(50),
1ELEMNTS(15)
COMMON /BLK3/X(100),Y(100),A(100,15),C(100),SF(100),CHEM(100,3),
1DF(100,3),DEL(100),STR(100,3),STR2(100,3),XK(100),CNC(100)
COMMON /BLK6/MAJOR(100),ITRACE(100)
COMMON /BLK7/M, NMAJOR, NTRACE, NN, XB, YB, T, PP, LAMDA, CP, ITNUM, TRACMX,
1CONCMN, CSTART, NORMAJ, NRUNS, LINE, LAST, KIP, NPP, ITP, IOT, TX, CURPLT
DIMENSION NA(15), NAM(15), NF(20), ICH(100,3), IDEL(100), ISTR(100,3),
1ISTR2(100,3), IXX(15)
EQUIVALENCE (XNA(1),NA(1)),(XNAM(1),NAM(1)),(GF(1),NF(1)),
1(CHEM(1),ICH(1)),(DEL(1),IDEL(1)),(STR(1),ISTR(1)),(STR2(1),ISTR2(
21)),(CURPLT,NURPLT),(BL,IBL),(XX(1),IXX(1))
DOUBLE PRECISION R,P,BAL,B,X,Y,A,C,SF,DEL,XB,YB,LAMDA
DOUBLE PRECISION DEL1,DEL2,AI,BI,CI
DATA RG/1.9864/
C WRITE TITLE, PAGE NUMBER, PP AND T
NPP=NPP+1
WRITE(IOT,300) (TITLE(I),I=1,12),NPP
IF(PP.LT.0.1) GO TO 5
WRITE(IOT,301) PP,T
GO TO 10
5 WRITE(IOT,302) PP,T
C COMPUTE FREE ENERGIES OF ALL CHEMICAL COMPOUNDS FOR A CURRENT
C TEMPERATURE SYSTEM
10 D21=TT(2)-TT(1)
D32=TT(3)-TT(2)
D31=TT(3)-TT(1)
S23=TT(2)+TT(3)
S12=TT(1)+TT(2)
DO 15 I=1,NN
DEL1=(DF(I,2)-DF(I,1))/D21
DEL2=(DF(I,3)-DF(I,2))/D32
AI=(DEL2-DEL1)/D31
BI=(DEL1*S23-DFL2*S12)/D31
CI=DF(I,1)-(AI*TT(1)+BI)*TT(1)
FOUT=AI*T+BI*T+CI
C WRITE OUT NAME OF CHEMICAL SPECIES AND ITS FREE ENERGY
WRITE(IOT,303) (CHEM(I,J),J=1,3),FOUT
C COMPUTE C(I) FOR ALL COMPOUNDS
15 C(I)=(1000.* (AI*T+BI*CI/T))/RG+DLOG(PP)
RETURN
C
C FORMAT SPECIFICATION
C
300 FORMAT(1H15X,12A6,10X,5H PAGE,I4)
301 FORMAT(1H017X,32H FREE ENERGY(DF) OF COMPOUNDS AT/6X,11H PRESSURE
1=F5.1,24H ATM AND TEMPERATURE =F7.2,7H KELVIN/1H011X,5H NAME,7X,
26H PHASE,15X,12H FREE ENERGY//)
302 FORMAT(1H017X,32H FREE ENERGY(DF) OF COMPOUNDS AT/6X,10H PRESSURE=
1E8.2,21H ATM AND TEMPERATURE=F7.2,7H KELVIN/1H011X,5H NAME,7X,6H P
2HASE,15X,12H FREE ENERGY//)
303 FORMAT(10X,3A6,18X,F9.3)
END

C SUBROUTINE CONC OF CHEM-EQ SYSTEM
C COMPUTES FREE ENERGIES OF ELEMENTS AND CONCENTRATIONS OF COMPOUNDS
C IN MASS BALANCE (MAJOR COMPOUNDS)
C CALLS SUBROUTINES LINEQ, PRINT, PRINT2
C
SUBROUTINE CONC
COMMON /BLK1/XNA(15),XNAM(15),R(17,17),P(16),BAL(15),NUM(16),B(15)
COMMON /BLK2/TITLE(12),GF(20),TT(3),XX(15),AF(50),AELE(50),
1ELEMNTS(15)
COMMON /BLK3/X(100),Y(100),A(100,15),C(100),SF(100),CHEM(100,3),

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1DF(100,3),DEL(100),STR(100,3),STR2(100,3),XK(100),CNC(100)
COMMON /BLK6/MAJOR(100),ITRACE(100)
COMMON /BLK7/M,NMAJOR,NTRACE,NN,XB,YB,T,PP,LAMDA,CP,ITNUM,TRACMX,
ICONCMN,CSTART,NORMAJ,NRUNS,LINE+LAST,KIP,NPP,ITP,IOT,TX,CURPLT
DIMENSION NA(15),NAM(15),NF(20),ICH(100,3),IDEL(100),ISTR(100,3),
ISTR2(100,3),IXX(15)
EQUIVALENCE (XNA(1),NA(1)),(XNAM(1),NAM(1)),(GF(1),NF(1)),
1(CHEM(1),ICH(1)),(DEL(1),IDEL(1)),(STR(1),ISTR(1)),(STR2(1),ISTR2(1))
DOUBLE PRECISION R,P,BAL,B,X,Y,A,C,SF,DEL,XB,YB,LAMDA
DOUBLE PRECISION LAM,SUM,DB,DELT,ARG
C INITIALIZE IT, LINE, M1, M2 AND BAL(I)
      IT=0
      LINE=0
      M1=M+1
      M2=M+2
      DO 5 I=1,M
      5 BAL(I)=0.
C COMPUTE SF(I) FOR ALL MAJOR COMPOUNDS AND B(J) FOR ALL ELEMENTS
      10 DO 15 I=1,NMAJOR
          IND=MAJOR(I)
      15 SF(IND)=Y(IND)*(C(IND)+DLOG(Y(IND)/YB))
          DO 20 J=1,M
          B(J)=0
          DO 20 I=1,NMAJOR
          IND=MAJOR(I)
      20 B(J)=B(J)+A(IND,J)*Y(IND)
C FIND COEFFICIENTS OF M+1 LINEAR EQUATIONS
      DO 25 J=1,M
      R(M1,J)=B(J)
      25 R(J,M1)=B(J)
      R(M1,M1)=0.0
      DO 35 J=1,M
      KL=J
      DO 35 K=KL,M
      R(J,K)=0.0
      DO 30 I=1,NMAJOR
      IND=MAJOR(I)
      30 R(J,K)=A(IND,J)*A(IND,K)*Y(IND)+R(J,K)
      35 R(K,J)=R(J,K)
      DO 40 J=1,M
      R(J,M2)=0.0
      DO 40 I=1,NMAJOR
      IND=MAJOR(I)
      40 R(J,M2)=R(J,M2)-A(IND,J)*SF(IND)
      R(M1,M2)=0.0
      DO 45 I=1,NMAJOR
      IND=MAJOR(I)
      - 45 R(M1,M2)=R(M1,M2)-SF(IND)
C CALL SUBROUTINE LINEQ TO SOLVE LINEAR EQUATIONS
      CALL LINEQ(R,P,M1,LINE,IOT)
C IF LINE IS 1 (NO SOLUTIONS BECAUSE DIAGONAL ELEMENT VANISHED),
C RETURN TO MAIN PROGRAM
      IF(LINE-1) 55,50,55
      50 RETURN
C COMPUTE NEXT APPROXIMATION TO CONCENTRATIONS OF MAJOR COMPOUNDS
      55 XB=YB*(P(M1)+1.0)
          DO 65 I=1,NMAJOR
          IND=MAJOR(I)
          SUM=0.0
          DO 60 J=1,M
          60 SUM=SUM+P(J)*A(IND,J)
          65 X(IND)=-SF(IND)+Y(IND)*XB/YB+SUM*Y(IND)
C
C PROCEED FOLLOWING STEPS (THROUGH STATEMENT NUMBER 130) FOR A
C CONVERGENCE GUARANTEE
C
          LAMDA=1.
          FRE=0.0
          DO 80 I=1,NMAJOR
          IND=MAJOR(I)
C COMPUTE TOTAL FREE ENERGY
          FRE=FRE+SF(IND)

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```

DEL(IND)=X(IND)-Y(IND)
IF(X(IND)) 70,70,80
70 LAM=-Y(IND)/DEL(IND)
IF(LAMDA-LAM) 80,80,75
75 LAMDA=LAM
80 CONTINUE
LAM=LAMDA
DB=0.0
DO 85 I=1,NMAJOR
IND=MAJOR(I)
DEL(IND)=DEL(IND)*LAMDA
X(IND)=Y(IND)+DEL(IND)
85 DB=DB+DEL(IND)
IF(ABS(P(M1))-0.003) 130,90,90
90 LAMDA=1.0
ITZ=0
95 DELT=0.0
100 DO 105 I=1,NMAJOR
IND=MAJOR(I)
ARG=(Y(IND)+LAMDA*DEL(IND))/(YB+LAMDA*DB)
IF(ARG.EQ.0.0) GO TO 105
DELT=DELT+DEL(IND)*(C(IND)+DLOG(ARG))
105 CONTINUE
ITZ=ITZ+1
IF(ITZ-2) 110,110,120
110 IF(DELT) 120,115,115
115 LAMDA=.5*LAMDA
GO TO 95
120 DO 125 I=1,NMAJOR
IND=MAJOR(I)
125 X(IND)=Y(IND)+LAMDA*DEL(IND)
LAMDA=LAMDA*LAM
130 CALL PRINT
C CHECK IF CONCENTRATIONS AND ELEMENTAL FREE ENERGIES CONVERGED
C IF SO, CALL SUBROUTINE PRINT2 AND RETURN
C OTHERWISE PROCEED TO NEXT ITERATION
DO 135 I=1,NMAJOR
IND=MAJOR(I)
IF(ABS(DEL(IND)/X(IND))-CP) 135,135,140
135 CONTINUE
DO 136 I=1,M
IF(ABS((P(I)-BAL(I))/P(I))-CP) 136,136,140
136 CONTINUE
CALL PRINT2(IT,FRE,IOT)
RETURN
140 YB=0.
DO 145 J=1,M
145 BAL(J)=P(J)
C IF CONCENTRATION OF A MAJOR COMPOUND IS LESS THAN CONCMN REMOVE THIS
C FROM MASS BALANCE AND MAKE IT A TRACE COMPONENT
150 IL=1
155 DO 160 I=IL,NMAJOR
IND=MAJOR(I)
IF(X(IND).LT.CONCMN) GO TO 165
160 CONTINUE
GO TO 170
165 IF(NMAJOR.LE.M) GO TO 170
NTRACE=NTRACE+1
ITRACE(NTRACE)=IND
MAJOR(I)=MAJOR(NMAJOR)
MAJOR(NMAJOR)=0
NMAJOR=NMAJOR-1
IF(I.GT.NMAJOR) GO TO 170
IL=I
GO TO 155
C COMPUTE Y(I) AND YB FOR NEXT ITERATION
170 DO 175 I=1,NMAJOR
IND=MAJOR(I)
Y(IND)=X(IND)
175 YB=YB+Y(IND)
IT=IT+1
C IF SOLUTION IS NOT OBTAINED WITHIN ITNUM ITERATIONS SET LINE=1, WRITE
C OUT INFORMATION AND RETURN
IF(IT-ITNUM) 10,180,180

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```

180 WRITE(IOT,500) ITNUM
    LINE=1
    CALL PRINT2(IT,FRE,IOT)
C
C FORMAT SPECIFICATION
C
500 FORMAT(1H05X,40H CONCENTRATIONS HAVE NOT CONVERGED AFTER,I3,54H IT
1ERATIONS. TRY AGAIN WITH BETTER INITIAL CONDITIONS.)
    RETURN
    END

C
C SUBROUTINE LINEQ OF CHEM-EQ SYSTEM
C LINEQ SOLVES A SYSTEM OF N LINEAR EQUATIONS  A(I,J)*X(J)+A(I,N+1)=0
C THE SOLUTIONS APPEAR IN X(N)
C
SUBROUTINE LINEQ(A2,X,N,LINE,IOT)
DIMENSION A2(17,17),X(16),A(17,17),B(16)
DOUBLE PRECISION A2,X,A,B,FAC,SUM
NH=N+1
NL=N-1
DO 10 I=1,N
DO 5 J=1,N
5 A(I,J)=A2(I,J)
10 A(I,NH)=-A2(I,NH)
DO 40 I=1,NL
I1=I+1
C REARRANGE EQUATIONS IF DIAGONAL ELEMENT VANISHES
IF(A(I,I)) 35,15,35
15 DO 30 KK=I1,N
IF(A(KK,I)) 20,30,20
20 DO 25 L=1,NH
B(L)=A(I,L)
A(I,L)=A(KK,L)
25 A(KK,L)=B(L)
GO TO 35
30 CONTINUE
GO TO 45
C ELIMINATE UNKNOWNSS
35 DO 40 J=I1,N
FAC=A(J,I)/A(I,I)
DO 40 K=I1,NH
40 A(J,K)=A(J,K)-A(I,K)*FAC
IF(A(N,N)) 50,45,50
45 WRITE(IOT,400) I
LINE=1
RETURN
C SOLVE FOR UNKNOWNSS
50 B(N)=A(N,NH)/A(N,N)
DO 60 II=2,N
J=N-II+1
SUM=0.
JJ=J+1
DO 55 K=JJ,N
55 SUM=B(K)*A(J,K)+SUM
60 B(J)=(A(J,NH)-SUM)/A(J,J)
DO 65 I=1,N
65 X(I)=B(I)
400 FORMAT(1H05X,29H DIAGONAL ELEMENT IN EQUATION I2,9H VANISHED)
RETURN
END

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```

C SUBROUTINE PRINT OF CHEM-EQ SYSTEM
C PRESENTLY A DUMMY ROUTINE
C
C      SUBROUTINE PRINT
C      RETURN
C      END

C
C SUBROUTINE PRINT2 OF CHEM-EQ SYSTEM
C PRINT OUT TOTAL FREE ENERGY AND NUMBER OF ITERATIONS MADE
C
C      SUBROUTINE PRINT2(IT,FRE,IOT)
C      WRITE(IOT,500) FRE
C      WRITE(IOT,501) IT
500 FORMAT(1H05X,20H TOTAL FREE ENERGY =F13.6)
501 FORMAT(1H05X,I2,44H ITERATIONS WERE MADE TO OBTAIN THE SOLUTION)
      RETURN
      END

C
C SUBROUTINE TCONC OF CHEM-EQ SYSTEM (PRINT ROUTINE)
C COMPUTES CONCENTRATIONS OF ALL COMPOUNDS, STORES NECESSARY ITEMS
C FOR A PRINT OUT OF TRIANGULAR DIAGRAMS AND PRINTS OUT ELEMENTAL
C FREE ENERGIES AND CONCENTRATIONS OF COMPOUNDS
C
C      SUBROUTINE TCONC
COMMON /BLK1/XNA(15),XNAM(15),R(17,17),P(16),BAL(15),NUM(16),B(15),
COMMON /BLK2/TITLE(12),GF(20),TT(3),XX(15),AF(50),AELE(50),
1FLEMTS(15)
COMMON /BLK3/X(100),Y(100),A(100,15),C(100),SF(100),CHEM(100,3),
1DF(100,3),DEL(100),STR(100,3),STR2(100,3),XK(100),CNC(100)
COMMON /BLK5/CPRT(4000)
COMMON /BLK6/MAJOR(100),ITRACE(100)
COMMON /BLK7/M,NMAJOR,NTRACE,NN,XB,YB,T,PP,LAMDA,CP,ITNUM,TRACMX,
1CONCMN,CSTART,NORMAJ,NRUNS,LINE,LAST,KIP,NPP,ITP,IOT,ITX,CURPLT
COMMON /BLK9/NR
DIMENSION NA(15),NAM(15),NF(20),ICH(100,3),IDEL(100),ISTR(100,3),
1ISTR2(100,3),IXX(15)
DIMENSION NCPRT(4000)
EQUIVALENCE (XNA(1),NA(1)),(XNAM(1),NAM(1)),(GF(1),NF(1)),
1(CHEM(1),ICH(1)),(DEL(1),IDEL(1)),(STR(1),ISTR(1)),(STR2(1),ISTR2(
21)),(CURPLT,NURPLT),(BL,IBL),(XX(1),IXX(1))
EQUIVALENCE (CPRT(1),NCPRT(1))
DOUBLE PRECISION R,P,BAL,B,X,Y,A,C,SF,DEL,XB,YB,LAMDA
DOUBLE PRECISION SUM,ARG
DATA DATA1,DATA2,DATA3,DATA4,DATA5,DATA6/5H(50X,,3HI5,,5H3XA2,,,
14HIH+,,3HI5),5H3XA2/
C COMPUTE CONCENTRATIONS OF ALL COMPOUNDS
K5=0
DO 10 I=1,NN
SUM=0.
DO 5 J=1,M
5 SUM=SUM+A(I,J)*P(J)
ARG=-C(I)+SUM
IF(ARG.GT.88.0) ARG=88.0
Y(I)=XB*DEXP(ARG)
10 CONTINUE
C INITIALIZE LINE TO ZERO. CHECK IF THERE ARE ANY TRACE COMPOUNDS
C WITH CONCENTRATION GREATER THAN TRACMX. IF SO, MAKE THEM MAJOR
C COMPOUNDS, ADJUST NMAJOR AND NTRACE, SET LINE TO 1 AND RETURN
LINE=0
IL=1
15 DO 20 I=IL,NTRACE
IND=ITRACE(I)
IF(Y(IND).GT.TRACMX) GO TO 25
20 CONTINUE
GO TO 30

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25 WRITE(IOT,600) (CHEM(IND,J),J=1,3),Y(IND)
NMAJOR=NMAJOR+1
MAJOR(NMAJOR)=IND
Y(IND)=CSTART
ITRACE(I)=ITRACE(NTRACE)
ITRACE(NTRACE)=0
NTRACE=NTRACE-1
IL=1
LINE=1
IF(I.GT.NTRACE) GO TO 30
GO TO 15
30 IF(LINE.EQ.1) RETURN
C CHECK IF THERE ARE ANY MAJOR COMPOUNDS WITH CONCENTRATION LESS THAN
C CONCMN. IF SO, MAKE THEM TRACE COMPOUNDS, ADJUST NMAJOR AND NTRACE
C SFT LINE TO 1 AND RETURN
IL=1
35 DO 40 I=IL,NMAJOR
IND=MAJOR(I)
IF(Y(IND).LT.CONCMN) GO TO 45
40 CONTINUE
GO TO 50
45 IF(NMAJOR.LE.M) GO TO 50
WRITE(IOT,601) (CHEM(IND,J),J=1,3),Y(IND)
NTRACE=NTRACE+1
ITRACE(NTRACE)=IND
MAJOR(I)=MAJOR(NMAJOR)
MAJOR(NMAJOR)=0
NMAJOR=NMAJOR-1
IL=1
LINE=1
IF(I.GT.NMAJOR) GO TO 50
GO TO 35
50 IF(LINE.EQ.1) RETURN
C WRITE TITLE, PAGE NUMBER, PP AND T
55 NPP=NPP+1
WRITE(IOT,602) (TITLE(I),I=1,12),NPP
IF(PP.LT.0.1) GO TO 56
WRITE(IOT,603) PP,T
GO TO 57
56 WRITE(IOT,624) PP,T
C COMPUTE INDEX NUMBER OF EACH ELEMENT ON THE BASIS OF C TO BE 100
57 DO 60 I=1,M
IF(NAM(I)-IXX(1)) 60,65,60
60 CONTINUE
I=M
65 XSTD=B(I)
70 DO 75 I=1,M
CNC(I)=B(I)/XSTD
75 IDEL(I)=CNC(I)*100.+5
C FORM VARIABLE FORMATS TO PRINT OUT NAMES OF ELEMENTS AND THEIR INDEX
C NUMBERS. ALSO, PRINT OUT THOSE NAMES AND INDEX NUMBERS
K3=1
DO 90 K1=2,25
DO 80 K2=1,M
IF(IXX(K1)-NAM(K2)) 80,85,80
80 CONTINUE
GO TO 90
85 K3=K3+1
NUM(K3)=IDEL(K2)
ELEMNTS(K3)=XX(K1)
90 CONTINUE
IF(K5) 105,95,105
95 AF(1)=DATA1
AELE(1)=DATA1
K5=1
DO 100 K1=3,M
K5=K5+1
AF(K5)=DATA2
AELE(K5)=DATA3
K5=K5+1
AF(K5)=DATA4
100 AELE(K5)=DATA4

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```

K5=K5+1
AF(K5)=DATA5
AELE(K5)=DATA6
105 WRITE(IOT,AELE) (ELEMTS(I),I=2,M)
      WRITE(IOT,AF) (NUM(I),I=2,M)
C COMPUTE MOLE FRACTIONS OF C, H, AND O AND PRINT OUT
      BB=0.
      DO 140 J=1,M
      NMJ=NAM(J)
      IF(NMJ-IXX(1)) 115,110,115
110  CNC(1)=B(J)
      GO TO 135
115 IF(NMJ-IXX(2)) 125,120,125
120  CNC(2)=B(J)
      GO TO 135
125 IF(NMJ-IXX(4)) 140,130,140
130  CNC(3)=B(J)
135  BB=BB+B(J)
140 CONTINUE
      DO 145 J=1,3
145  CNC(J)=CNC(J)/BB
      WRITE(IOT,604) (CNC(I),I=1,3)
C STORE MOLE FRACTIONS OF C, H, AND O AND FREE ENERGIES OF ELEMENTS
C IN CPRT(I). ALSO, PRINT OUT
      IF(NR=70) 150,150,165
150  K2=(NR-1)*(NN+M+3)
      DO 155 I=1,3
      K2=K2+1
155  CPRT(K2)=CNC(I)
      DO 160 I=1,M
      K2=K2+1
160  CPRT(K2)=P(I)
165  WRITE(IOT,605)
      DO 170 J=1,M
170  WRITE(IOT,606) XNAM(J),B(J),P(J)
      WRITE(IOT,607) XB
      WRITE(IOT,608)
C PRINT OUT NAMES AND CONCENTRATIONS OF MAJOR COMPOUNDS
      DO 175 I=1,NMAJOR
      IND=MAJOR(I)
175  WRITE(IOT,609) (CHEM(IND,J),J=1,3),X(IND),Y(IND)
C STORE CONCENTRATIONS OF ALL COMPOUNDS IN XK(I). CALL SUBROUTINE
C ORDRFD TO ARRANGE TRACE COMPOUNDS IN DESCENDING ORDER OF THEIR
C CONCENTRATIONS
      DO 195 I=1,NN
      IF(I.GT.NMAJOR) GO TO 185
      IND=MAJOR(I)
      IDEL(I)=IND
      GO TO 190
185  ISUB=I-NMAJOR
      IND=ITRACE(ISUB)
      IDEL(I)=IND
190  XK(I)=Y(IND)
195 CONTINUE
      IF(NN-NMAJOR) 315,225,196
196  WRITE(IOT,610)
      CALL ORDRFD(XK(NMAJOR+1),IDEL(NMAJOR+1),NTRACE)
C PRINT OUT CONCENTRATIONS OF TRACE COMPOUNDS
      WRITE(IOT,611)
      NI=NMAJOR+1
      NL=40-M
      GO TO 205
200  NPP=NPP+1
      WRITE(IOT,612) NPP
      WRITE(IOT,611)
      NI=NI+1
      NL=NI+52
205  IF(NL>NN) 215,215,210
210  NL=NN
215  DO 220 I=NI,NL
      ISUB=I-NMAJOR
      IND=ITRACE(ISUB)
      IND2=IDEL(I)

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220 WRITE(IOT,613) (CHEM(IND,J),J=1,3),Y(IND),(CHEM(IND2,J),J=1,3),XK(
11)
   IF(NL-NN) 200,225,225
C WRITE TITLE, PAGE NUMBER, PP AND T
225 NPP=NPP+1
230 WRITE(IOT,602) (TITLE(I),I=1,12),NPP
   IF(PP.LT.0.1) GO TO 231
   WRITE(IOT,603) PP,T
   GO TO 232
231 WRITE(IOT,624) PP,T
C PRINT OUT INDEX NUMBERS OF ELEMENTS AND MOLE FRACTIONS OF C, H, AND O
232 WRITE(IOT,AELE) (ELEMTS(I),I=2,M)
   WRITE(IOT,AF) (NUM(I),I=2,M)
   WRITE(IOT,604) (CNC(I),I=1,3)
   WRITE(IOT,605)
   DO 235 J=1,M
235 WRITE(IOT,606) XNAM(J),B(J),P(J)
   WRITE(IOT,620)
C CALL SUBROUTINE ORDRFD TO ARRANGE ALL COMPOUNDS IN A DESCENDING ORDER
C OF THEIR CONCENTRATIONS
   CALL ORDRFD(XK,IDELEM,NN)
C NORMALIZE CONCENTRATIONS OF ALL COMPOUNDS, STORE THEM IN CPRT(I),
C AND PRINT OUT
   DO 240 I=1,NMAJOR
     IND=MAJOR(I)
240 Y(IND)=X(IND)
   DO 255 I=1,NN
     IND=IDELEM(I)
   DO 245 J=1,NN
     IF(J.EQ.IND) GO TO 250
245 CONTINUE
   J=NN
250 XK(J)=XK(I)
255 CONTINUE
   DO 265 I=1,NN
260 CNC(I)=XK(I)/XB
265 XK(I)=X(I)/XB
   NI=1
   NL=43-M
   GO TO 275
270 NPP=NPP+1
   WRITE(IOT,612) NPP
   NI=NL+1
   NL=NI+52
275 IF(NL-NN) 285,285,280
280 NL=NN
285 WRITE(IOT,611)
   IF(NR-70) 290,290,305
290 K2=(NR-1)*(NN+M+3)+M+3
   DO 300 I=1,NN
     K2=K2+1
300 CPRT(K2)=XK(I)
305 DO 310 I=NI,NL
   IND=IDELEM(I)
310 WRITE(IOT,613) (CHEM(I,J),J=1,3),XK(I),(CHEM(IND,J),J=1,3),CNC(I)
   IF(NL-NN) 270,315,315
315 RETURN
C
C FORMAT SPECIFICATIONS
C
600 FORMAT(1H 5X,16H TRACE COMPOUND 3A6,29H HAS EXCESSIVE CONCENTRATION
   IN E9.3,38H, MAKE THIS A MAJOR COMPOUND AND REDO.)
601 FORMAT(1H 5X,16H MAJOR COMPOUND 3A6,29H HAS TOO SMALL CONCENTRATION
   IN E9.3,38H, MAKE THIS A TRACE COMPOUND AND REDO.)
602 FORMAT(1H15X,12A6,10X,5H PAGE,I4)
603 FORMAT(1H05X,9H PRESSURE,5X,12H TEMPERATURE/ 5X,F6.1,4H ATM,6X,F7.
   12,7H KELVIN)
624 FORMAT(1H05X,9H PRESSURE,5X,12H TEMPERATURE/5X,E9.2,4H ATM,3X,F7.2
   1,7H KELVIN)
604 FORMAT(1H035X,14H MOLE FRACTION,4X1HC,6X,1HH,6X,1H0/52X,2(F5.4,1H-
   1,1X),F5.4)
605 FORMAT(1H05X,7HELEMENT,4X,5HMOLES,8X,6HF/MOLE)
606 FORMAT(8X,A2,3X,F10.5,3X,F10.5)

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607 FORMAT(1H011X,7HSPECIES,10X,20HCOMPOSITION IN MOLES,F6.2,12H TOTAL
1 MOLES)
608 FORMAT(29X,11H(MASS BAL.),7X,15H(F OF ELEMENTS))
609 FORMAT(7X,3A6,3X,F10.6,11X,E10.4)
610 FORMAT(1H05X,16HTRACE COMPONENTS)
611 FORMAT(6X,12HNORMAL ORDER,31X,22HDECREASING COMPOSITION//)
612 FORMAT(1H187X,5H PAGE,I4)
613 FORMAT(7X,3A6,3X,E10.4,11X,3A6,3X,E10.4)
620 FORMAT(1H011X,7HSPECIES,10X,38HMOLE FRACTION COMPOSITION (NORMALIZ
1ED))
END

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C SUBROUTINE TCONC OF CHEM-EQ SYSTEM (NO PRINT ROUTINE)
C COMPUTES CONCENTRATIONS OF ALL COMPOUNDS, STORES NECESSARY ITEMS
C FOR A PRINT OUT OF TRIANGULAR DIAGRAMS
C
SUBROUTINE TCONC
COMMON /BLK1/XNA(15),XNAM(15),R(17,17),P(16),BAL(15),NUM(16),B(15)
COMMON /BLK2/TITLE(12),GF(20),TT(3),XX(15),AF(50),AELE(50),
1ELEMTS(15)
COMMON /BLK3/X(100),Y(100),A(100,15),C(100),SF(100),CHEM(100,3),
1DF(100,3),DEL(100),STR(100,3),STR2(100,3),XK(100),CNC(100)
COMMON /BLK5/CPRT(4000)
COMMON /BLK6/MAJOR(100),ITRACE(100)
COMMON /BLK7/M,NMAJOR,NTRACE,NN,XB,YB,T,PP,LAMDA,CP,ITNUM,TRACMX,
1CONCMN,CSTART,NORMAJ,NRUNS,LINE,LAST,KIP,NPP,ITP,IOT,TX,CURPLT
COMMON /BLK9/NR
DIMENSION NA(15),NAM(15),NF(20),ICH(100,3),IDEL(100),ISTR(100,3),
1ISTR2(100,3),IXX(15)
DIMENSION NCPRT(4000)
EQUIVALENCE (XNA(1),NA(1)),(XNAM(1),NAM(1)),(GF(1),NF(1)),
1(CHEM(1),ICH(1)),(DEL(1),IDEL(1)),(STR(1),ISTR(1)),(STR2(1),ISTR2(
21)),(CURPLT,NURPLT),(BL,IBL),(XX(1),IXX(1))
EQUIVALENCE (CPRT(1),NCPRT(1))
DOUBLE PRECISION R,P,BAL,B,X,Y,A,C,SF,DEL,XB,YB,LAMDA
DOUBLE PRECISION SUM,ARG
DATA DATA1,DATA2,DATA3,DATA4,DATA5,DATA6/5H(50X,,3H15,,5H3XA2,,14H1H--,,3H15),5H3XA2)/
C COMPUTE CONCENTRATIONS OF ALL COMPOUNDS
K5=0
DO 10 I=1,NN
SUM=0.
DO 5 J=1,M
5 SUM=SUM+A(I,J)*P(J)
ARG=-C(I)+SUM
IF(ARG.GT.88.0) ARG=88.0
Y(I)=XB*DEXP(ARG)
10 CONTINUE
C INITIALIZE LINE TO ZERO. CHECK IF THERE ARE ANY TRACE COMPOUNDS
C WITH CONCENTRATION GREATER THAN TRACMX. IF SO, MAKE THEM MAJOR
C COMPOUNDS, ADJUST NMAJOR AND NTRACE, SET LINE TO 1 AND RETURN
LINE=0
IL=1
15 DO 20 I=IL,NTRACE
IND=ITRACE(I)
IF(Y(IND).GT.TRACMX) GO TO 25
20 CONTINUE
GO TO 30
25 WRITE(IOT,600) (CHEM(IND,J),J=1,3),Y(IND)
NMAJOR=NMAJOR+1
MAJOR(NMAJOR)=IND
Y(IND)=CSTART
ITRACE(I)=ITRACE(NTRACE)
ITRACE(NTRACE)=0
NTRACE=NTRACE-1
IL=I
LINE=1

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        IF(I.GT.NTRACE) GO TO 30
        GO TO 15
30 IF(LINE.EQ.1) RETURN
C CHECK IF THERE ARE ANY MAJOR COMPOUNDS WITH CONCENTRATION LESS THAN
C CONCMN. IF SO, MAKE THEM TRACE COMPOUNDS, ADJUST NMAJOR AND NTRACE
C SET LINE TO 1 AND RETURN
        IL=1
35 DO 40 I=IL,NMAJOR
        IND=MAJOR(I)
        IF(Y(IND).LT.CONCMN) GO TO 45
40 CONTINUE
        GO TO 50
45 IF(NMAJOR.LE.M) GO TO 50
        WRITE(IOT,601) (CHEM(IND,J),J=1,3),Y(IND)
        NTRACE=NTRACE+1
        ITRACE(ITRACE)=IND
        MAJOR(I)=MAJOR(NMAJOR)
        MAJOR(NMAJOR)=0
        NMAJOR=NMAJOR-1
        IL=I
        LINE=1
        IF(I.GT.NMAJOR) GO TO 50
        GO TO 35
50 IF(LINE.EQ.1) RETURN
C COMPUTE MOLE FRACTIONS OF C, H, AND O
        BB=0.
        DO 140 J=1,M
        NMJ=NAM(J)
        IF(NMJ-IXX(1)) 115,110,115
110 CNC(1)=B(J)
        GO TO 135
115 IF(NMJ-IXX(2)) 125,120,125
120 CNC(2)=B(J)
        GO TO 135
125 IF(NMJ-IXX(4)) 140,130,140
130 CNC(3)=B(J)
135 BB=BB+B(J)
140 CONTINUE
        DO 145 J=1,3
145 CNC(J)=CNC(J)/BB
C STORE MOLE FRACTIONS OF C, H, AND O AND FREE ENERGIES OF ELEMENTS
C IN CPRT(I).
        IF(NR=70) 150,150,165
150 K2=(NR-1)*(NN+M+3)
        DO 155 I=1,3
        K2=K2+1
155 CPRT(K2)=CNC(I)
        DO 160 I=1,M
        K2=K2+1
160 CPRT(K2)=P(I)
C STORE CONCENTRATIONS OF ALL COMPOUNDS IN XK(I).
165 DO 195 I=1,NN
        IF(I.GT.NMAJOR) GO TO 185
        IND=MAJOR(I)
        IDEL(I)=IND
        GO TO 190
185 ISUB=I-NMAJOR
        IND=ITRACE(ISUB)
        IDEL(I)=IND
190 XK(I)=Y(IND)
195 CONTINUE
        DO 255 I=1,NN
        IND=IDEL(I)
        DO 245 J=1,NN
        IF(J.EQ.IND) GO TO 250
245 CONTINUE
        J=NN
250 X(J)=XK(I)
255 CONTINUE
C NORMALIZE CONCENTRATIONS OF ALL COMPOUNDS, STORE THEM IN CPRT(I)

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DO 265 I=1,NN
260 CNC(I)=XK(I)/XB
265 XK(I)=X(I)/XB
IF(NR>70) 290,290,315
290 K2=(NR-1)*(NN+M+3)+M+3
DO 300 I=1,NN
K2=K2+1
300 CPRT(K2)=XK(I)
315 RRETURN
C
C FORMAT SPECIFICATIONS
C
600 FORMAT(1H 5X,16H TRACE COMPOUND 3A6,29H HAS EXCESSIVE CONCENTRATIO
IN E9.3,38H, MAKE THIS A MAJOR COMPOUND AND REDO.)
601 FORMAT(1H 5X,16H MAJOR COMPOUND 3A6,29H HAS TOO SMALL CONCENTRATIO
IN E9.3,38H, MAKE THIS A TRACE COMPOUND AND REDO.)
END

C
C SUBROUTINE ORDRFD OF CHEM-EQ SYSTEM
C ARRANGES A LIST OF NUMBERS, X(I), INTO A DESCENDING ORDER
C ALSO, REORDERS AN ASSOCIATED LIST, L(I)
C
SUBROUTINE ORDRFD(X,L,J)
DIMENSION X(100),L(100)
IF(J.LE.1) RETURN
JL=J-1
DO 100 I=1,JL
KL=I+1
DO 50 K=KL,J
IF(X(I).GE.X(K)) GO TO 50
TEMP=X(I)
TEMP1=L(I)
X(I)=X(K)
L(I)=L(K)
X(K)=TEMP
L(K)=TEMP1
50 CONTINUE
100 CONTINUE
RETURN
END

C
C SUBROUTINE TABLE OF CHEM-EQ SYSTEM (PRINT ROUTINE)
C PRINTS OUT A TABLE OF SUMMARY OF RUNS
C
SUBROUTINE TABLE
COMMON /BLK1/XNA(15),XNAM(15),R(17,17),P(16),BAL(15),NUM(16),B(15)
COMMON /BLK2/TITLE(12),GF(20),TT(3),XX(15),AF(50),AELE(50),
1ELEMNTS(15)
COMMON /BLK3/X(100),Y(100),A(100,15),C(100),SF(100),CHEM(100,3),
1DF(100,3),DEL(100),STR(100,3),STR2(100,3),XK(100),CNC(100)
COMMON /BLK5/CPRT(4000)
COMMON /BLK7/M,NMAJOR,NTRACE,NN,XB,YB,T,PP,LAMDA,CP,ITNUM,TRACMX,
1CONCMN,CSTART,NORMAJ,NRUNS,LINE,LAST,KIP,NPP,ITP,IOT,TX,CURPLT
COMMON /BLK10/NUMRUN(9)
DIMENSION NCPRT(4000)
EQUIVALENCE (CPRT(1),NCPRT(1))
DOUBLE PRECISION R,P,BAL,B,X,Y,A,C,SF,DEL,XB,YB,LAMDA
DIMENSION XPRT(3),XPRT1(9)
C PRINT OUT RUN NUMBER, MOLE FRACTIONS OF C, H, AND O AND FREE ENERGIES
C OF ELEMENTS IN THAT RUN
INDEX=1
NSTEP=M+NN+3
M3=M+3
100 NPP=NPP+1
WRITE(IOT,1000) (TITLE(I),I=1,12),NPP
IF(PP.LT.0.1) GO TO 1
WRITE(IOT,1008) PP,T

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      GO TO 101
1  WRITE(IOT,1009) PP,T
101 GO TO (2+3,25,30),INDEX
2  WRITE(IOT,1001)
   I1=1
   I2=40
3  WRITE(IOT,1010) (XNAM(I),I=1,M)
   WRITE(IOT,1007)
   IF(I2.GT.NRUNS) I2=NRUNS
   DO 10 I=I1,I2
   IL=(I-1)*NSTEP
   JL=IL+4
   JH=JL+M-1
   DO 5 K=1,3
   IND=IL+K
5   XPRT(K)=CPRT(IND)*100.
   WRITE(IOT,1002) I,(XPRT(II),II=1,3),(CPRT(J),J=JL,JH)
10  CONTINUE
   IF(I2.GE.NRUNS) GO TO 11
   I1=I2+1
   I2=I1+44
   INDEX=2
   GO TO 100
11  NPOINT=0
C DETERMINE NUMBER OF POINTS SELECTED
   DO 15 I=1,9
   IF(NUMRUN(I).NE.0) NPOINT=NPOINT+1
15  CONTINUE
C PRINT OUT CONCENTRATIONS OF ALL COMPOUNDS IN THOSE SELECTED RUNS
   INDEX=3
   GO TO 100
25  IL=1
   IH=45
   WRITE(IOT,1004)
30  IF(NN.LT.IH) IH=NN
   WRITE(IOT,1005) (NUMRUN(I),I=1,NPOINT)
   WRITE(IOT,1007)
   GO TO 40
35  IL=IH+1
   IH=IL+49
   INDEX=4
   GO TO 100
40  DO 50 I=IL,IH
   DO 45 J=1,NPOINT
   ISUB=(NUMRUN(J)-1)*NSTEP+M3+I
   XPRT1(J)=CPRT(ISUB)
45  CONTINUE
   WRITE(IOT,1006) (CHEM(I,K),K=1,3),(XPRT1(J),J=1,NPOINT)
50  CONTINUE
   IF(NN.GT.IH) GO TO 35
   RETURN
1000 FORMAT(1H1,12A6,15X,5H PAGE,I4)
1001 FORMAT(//23X,24H TABLE. SUMMARY OF RUNS/1H029HA. FREE ENERGIES O
   1F ELEMENTS.)
1002 FORMAT(1X,I3,1X,3F6.1,5X,10F10.3)
1003 FORMAT(1H187X,5H PAGE,I4)
1004 FORMAT(1H055HB. CONCENTRATIONS OF THE COMPOUNDS IN THE TYPICAL RUN
   1S.)
1005 FORMAT(1H06X,10H COMPOUNDS,19X,15H CONCENTRATIONS//4X5H NAME,6X,6H
   1 PHASE,4X,4H RUN,I3,8(7X,I3))
1006 FORMAT(2X,3A6,5X,1P9E10.1)
1007 FORMAT(1H0)
1008 FORMAT(1H01H PRESSURE =F5.1,26H ATM AND TEMPERATURE =F7.2,7H
   1KELVIN//)
1009 FORMAT(1H01H PRESSURE =E8.2,26H ATM AND TEMPERATURE =F7.2,7H
   1KELVIN//)
1010 FORMAT(1H022H RUN MOLE PERCENTAGE,15X,23H FREE ENERGIES (F/MOLE)
   1/1H04H NO.3X,2H C,4X,2H H4X,2H O3X,10(8X,A2))
   END

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C SUBROUTINE TABLE OF CHEM-EQ SYSTEM (PUNCH ROUTINE)
C PUNCHES OUT INITIAL GUESS CARDS
C
SUBROUTINE TABLE
COMMON /BLK1/XNA(15),XNAM(15),R(17,17),P(16),BAL(15),NUM(16),B(15)
COMMON /BLK2/TITLE(12),GF(20),TT(3),XX(15),AF(50),AELE(50),
1ELEMTS(15)
COMMON /BLK3/X(100),Y(100),A(100,15),C(100),SF(100),CHEM(100,3),
1DF(100,3),DEL(100),STR(100,3),STR2(100,3),XK(100),CNC(100)
COMMON /BLK5/CPRT(4000)
COMMON /BLK7/M,NMAJOR,NTRACE,NN,XB,YB,T,PP,LAMDA,CP,ITNUM,TRACMX,
1CONCMN,CSTART,NORMAJ,NRUNS,LINE,LAST,KIP,NPP,ITP,IOT,ITX,CURPLT
COMMON /BLK10/NUMRUN(9)
DIMENSION NCPRT(4000)
EQUIVALENCE (CPRT(1),NCPRT(1))
DOUBLE PRECISION R,P,BAL,B,X,Y,A,C,SF,DEL,XB,YB,LAMDA
DIMENSION XPRT(20)
DIMENSION ID(3)
NPP=NPP+1
WRITE(IOT,1005) (TITLE(I),I=1,12),NPP
C FIND A MAXIMUM OF NUMBER OF COMPOUNDS WITH CONCENTRATION GREATER
C THAN OR EQUAL TO CSTART OF EACH RUN
NSTEP=M+NN+3
M3=M+3
KMAX=0
DO 10 I=1,NRUNS
JL=(I-1)*NSTEP+M3+1
JH=JL+NN-1
K=0
DO 5 J=JL,JH
5 IF(CPRT(J).GE.CSTART) K=K+1
IF(KMAX.LT.K) KMAX=K
10 CONTINUE
C PRINT OUT INFORMATIONS ABOUT INITIAL GUESS CARDS PUNCHED OUT
NCARD=(KMAX+1)/2
NTOTAL=NCARD*NRUNS
WRITE(IOT,1000) KMAX,KMAX,NCARD,NTOTAL
C PUNCH OUT INITIAL GUESS CARDS
DO 30 I=1,NRUNS
K=0
IL=(I-1)*NSTEP
C COMPUTE MOLE PERCENTAGE OF C, H AND O, AND PUNCH OUT THEM AS ID
DO 12 II=1,3
IND=IL+II
12 ID(II)=CPRT(IND)*100.+0.5
JL=IL+M3
DO 15 J=1,NN
ISUB=JL+J
IF(CPRT(ISUB).LT.CSTART) GO TO 15
K=K+1
DO 11 JJ=1,3
11 STR2(K,JJ)=CHEM(J,JJ)
XPRT(K)=CPRT(ISUB)
15 CONTINUE
IF(K.GT.KMAX) WRITE(IOT,1001) I,K,KMAX
DO 20 L=1,KMAX,2
ML=L
MH=ML+1
IF(MH.LE.K) GO TO 16
IF(ML.EQ.K) GO TO 17
IF(ML.GT.K) WRITE(7,1002) (ID(JJ),JJ=1,3)
GO TO 20
16 WRITE(7,1003) ((STR2(MM,JJ),JJ=1,3),XPRT(MM),MM=ML,MH),(ID(JJ),JJ=
11,3)
GO TO 20
17 WRITE(7,1004) (STR2(ML,JJ),JJ=1,3),XPRT(ML),(ID(JJ),JJ=1,3)
20 CONTINUE
30 CONTINUE
RETURN
C

```

```

C FORMAT SPECIFICATIONS
C
1000 FORMAT(1H0/1H010X,18H *** ATTENTION ***/1H015X,53H THIS JOB PRODUC
    1ES PUNCHED CARDS FOR INITIAL GUESSES./1H015X,53H WHEN THESE CARDS
    2ARE USED, MAKE THE VALUE OF NGUESS I2,1H*/17X,13H (I.E., PUNCH I3,
    352H IN COLUMNS BETWEEN 41 AND 50 OF THE CONSTANT CARD.)/1H0/1H015X
    417H THERE SHOULD BE I2,24H CARDS FOR EACH RUN AND I3,45H CARDS IN
    5TOTAL PUNCHED OUT WITH THIS SYSTEM.)
1001 FORMAT(1H0/1H010X,14H *** WRONG ***/1H015X,42H SOMETHING IS WRONG,
    1 BECAUSE WITH RUN NO. I2,29H, NUMBER OF GUESS COMPOUNDS (I2,4H) IS
    2/16X,49H GREATER THAN THE MAXIMUM PREVIOUSLY DETERMINED (I2,2H).)
1002 FORMAT(72X,3I2)
1003 FORMAT(2(3A6,F9.8,1X),16X,3I2)
1004 FORMAT(3A6,F9.8,45X,3I2)
1005 FORMAT(1H112A6,15X,5H PAGE,I4)
END

```

```

C SUBROUTINE TRIPRT OF CHEM-EQ SYSTEM
C PRINTS OUT TRIANGULAR DIAGRAM FOR EACH ELEMENT (FREE ENERGY) AND EACH
C COMPOUND (CONCENTRATION)
C PRINTS COMPLETE GRID DIAGRAM IF TX=1.0 AND A MAGNIFIED DIAGRAM IF
C TX IS GREATER THAN 1.0
C
SUBROUTINE TRIPRT
COMMON /BLK1/XNA(15),XNAM(15),R(17,17),P(16),BAL(15),NOM(16),B(15),
COMMON /BLK2/TITLE(12),GF(20),TT(3),XX(15),AF(50),AELE(50),
IELEMTS(15)
COMMON /BLK3/X(100),Y(100),A(100,15),C(100),SF(100),CHEM(100,3),
1DF(100,3),DEL(100),STR(100,3),STR2(100,3),XK(100),CNC(100)
COMMON /BLK5/CPRT(4000)
COMMON /BLK6/MAJOR(100),ITRACE(100)
COMMON /BLK7/M,NMAJOR,NTRACE,NN,XB,YB,T,PP,LAMDA,CP,ITNUM,TRACMX,
1CONCMN,CSTART,NORMAJ,NRUNS,LINE,LAST,KIP,NPP,ITP,IOT,TX,CURPLT
DIMENSION NA(15),NAM(15),NF(20),ICH(100,3),IDEL(100),ISTR(100,3),
1ISTR2(100,3),IXX(15)
DIMENSION NCPRT(4000)
EQUIVALENCE (XNA(1),NA(1)),(XNAM(1),NAM(1)),(GF(1),NF(1)),
1(CHEM(1),ICH(1)),(DEL(1),IDEL(1)),(STR(1),ISTR(1)),(STR2(1),ISTR2(1)),
1,(CURPLT,NURPLT),(BL,IBL),(XX(1),IXX(1))
EQUIVALENCE (CPRT(1),NCPRT(1))
DOUBLE PRECISION R,P,BAL,B,X,Y,A,C,SF,DEL,XB,YB,LAMDA
DIMENSION IPOS(4),IX(70),IY(70),IXPTX(30),
1IXPTY(30),FIXPTV(30),LVARX(10),LVARY(10),ILABX(10),ILABY(10),
2XVAR(10),IXC(25),IYC(25),KORT(25),QUANT(25),ORDR(25),LIST(25),
3VFOR(50),DIC(25),NCHAR(10),OUT(10)
DIMENSION YNAM(25)
DATA BLANK/0606060606060/,ZZZ/0777700000000/,FADD/5H00 DF/,STAR,
1CC,O,H/1H*,1HC,1HO,1HH/
DATA (DIC(I),I=1,21)/5H00000,5H00100,5H00200,5H00300,5H00400,
15H00500,5H00600,5H00700,5H00800,5H00900,5H00000,5H01000,5H02000,
25H03000,5H04000,5H05000,5H06000,5H07000,5H08000,5H09000,5H10000/
DATA (OUT(I),I=1,4)/3HA1,,5HE7.2,,3HA6,,3HA4,/
DATA (NCHAR(I),I=1,4)/1,7,6,4/
DATA CO2+H2O,CH4,CO/4HCO2*,4H H2O,4H*CH4,4H CO/
DATA FFOR/5H000X/,VFOR(1)/1H(/,VLAST/3H1X)/
C FORM YNAM(I) WHICH IS A STRING OF LETTERS WITH NAME OF ELEMENT
C FOLLOWED BY A BLANK AND LETTERS DF
K2=0
DO 5 I=1,M
    YNAM(I)=AND(ZZZ,XNAM(I))
5 YNAM(I)=OR(YNAM(I),FADD)
C PUT FIXED POINTS IN LISTS
DO 10 I=1,11
    IXPTX(I)=64+(I-1)*5
    IXPTY(I)=51-(I-1)*5
10 FIXPTV(I)=STAR
DO 15 I=1,10

```

```

IXPTX(I+11)=6+10*I
IXPTY(I+11)=51
15 FIXPTV(I+11)=STAR
IXPTX(22)=58
IXPTY(22)=1
FIXPTV(22)=CC
IXPTX(23)=3
IXPTY(23)=51
FIXPTV(23)=0
IXPTX(24)=108
IXPTY(24)=51
FIXPTV(24)=H
IXPTX(25)=72
IXPTY(25)=51
FIXPTV(25)=STAR
C PUT NAMES OF SIMPLE COMPOUNDS
ILABX(1)=20
ILABY(1)=34
XVAR(1)=CO2
ILABX(2)=68
ILABY(2)=51
XVAR(2)=H2O
ILABX(3)=96
ILABY(3)=41
XVAR(3)=CH4
ILABX(4)=27
ILABY(4)=26
XVAR(4)=CO
C PUT COORDINATES OF X AND Y WHERE NAME WILL BE PRINTED OUT
LVARX=10
LVARY=11
NSTEP=NN+M+3
IF(TX.LE.1.0) GO TO 22
C TX IS GREATER THAN 1.0. FIND SMALLEST VALUES OF C AND H FRACTIONAL
C COMPOSITION (ORG C AND ORGH)
ORG C=1000.
ORG H=1000.
DO 16 I=1,NRUNS
NCFCT=NSTEP*(I-1)+1
NHFCT=NCFCT+1
IF(CPRT(NCFCT).EQ.0.0.AND.CPRT(NHFCT).EQ.0.0.AND.CPRT(NHFCT+1).EQ.
10.0) GO TO 16
IF(CPRT(NHFCT).LT.ORG H) ORGH=CPRT(NHFCT)
IF(CPRT(NCFCT).LT.ORG C) ORGC=CPRT(NCFCT)
16 CONTINUE
C ADJUST C AND H CONCENTRATIONS RELATIVE TO ORGC AND ORGH AND
C SCALE BY A FACTOR TX
IFIXC=100.*ORG C
IFIXH=100.*ORG H
IORG C=TX*(100.*ORG C-FLOAT(IFIXC))-1.7
IORG H=TX*(100.*ORG H-FLOAT(IFIXH))-1.7
ORG C=FLOAT(IFIXC)+FLOAT(IORG C)/TX
ORG H=FLOAT(IFIXH)+FLOAT(IORG H)/TX
C COMPUTE IX AND IY (THE COORDINATES) OF EACH RUN
DO 18 I=1,NRUNS
NCFCT=NSTEP*(I-1)+1
NHFCT=NCFCT+1
IF(CPRT(NCFCT).EQ.0.0.AND.CPRT(NHFCT).EQ.0.0.AND.CPRT(NHFCT+1).EQ.
10.0) GO TO 17
IX(I)=(CPRT(NHFCT)*100.-ORG H)*TX+(50.*CPRT(NCFCT)-ORG C/2.)*TX+6.5
IY(I)=TX*(ORG C/2.-50.*CPRT(NCFCT))+51.5
GO TO 18
17 IX(I)=0
IY(I)=0
18 CONTINUE
GO TO 20
C TX=1.0. COMPUTE IX AND IY (THE COORDINATES) OF EACH RUN
22 DO 25 I=1,NRUNS
NCFCT=NSTEP*(I-1)+1
NHFCT=NCFCT+1

```

```

IF(CPRT(NCFCT).EQ.0.0.AND.CPRT(NHFCT).EQ.0.0.AND.CPRT(NHFCT+1).EQ.
10.0) GO TO 23
IX(I)=100.*CPRT(NHFCT)+50.*CPRT(NCFCT)+6.5
IY(I)=-50.*CPRT(NCFCT)+51.5
GO TO 25
23 IX(I)=0
IY(I)=0
25 CONTINUE
C
C PRINTING ROUTINE BEGINS HERE
C
20 K2=K2+1
C WRITE TITLE, PAGE NUMBER, PP AND T
NPP=NPP+1
WRITE(IOT,800) (TITLE(I),I=1,12),NPP
IF(PP.LT.0.1) GO TO 30
WRITE(IOT,801) PP,T
GO TO 35
30 WRITE(IOT,802) PP,T
C INITIALIZE LINE TO ZERO
35 LINE=0
C INCREASE LINE BY ONE AND FIND ITEMS TO BE PRINTED ON THAT LINE
C THERE WILL BE NUM ITEMS STORED IN QUANT(I) EACH WITH FORMAT TYPE
C KORMT(I) AND X COORDIANTE IXC(I)
45 LINE=LINE+1
NUM=0
C IF LINE=LVARX, STORE NAME OF ELEMENT OR COMPOUND IN QUANT(I) AND
C LVARX IN IXC(I)
IF(LVARX.EQ.LINE) GO TO 50
GO TO 60
50 NUM=NUM+3
IXC(NUM-2)=LVARX
IXC(NUM-1)=LVARX+6
IXC(NUM)=LVARX+12
KORMT(NUM-2)=3
KORMT(NUM-1)=3
KORMT(NUM)=3
IF(K2.LE.M) GO TO 55
QUANT(NUM-1)=YNAM(K2)
QUANT(NUM)=BLANK
C IF TX=1.0, SEARCH FOR SIMPLE COMPOUND NAMES APPEARING IN A COMPLETE
C GRID DIAGRAM
60 IF(TX.GT.1.0) GO TO 71
DO 70 I=1,4
IF(ILABY(I).NE.LINE) GO TO 70
NUM=NUM+1
IXC(NUM)=ILABX(I)
KORMT(NUM)=4
QUANT(NUM)=XVAR(I)
70 CONTINUE
C SEARCH SINGLE CHARACTERS
71 DO 80 I=1,25
IF(IXPTY(I).NE.LINE) GO TO 80
NUM=NUM+1
IXC(NUM)=IXPTX(I)
KORMT(NUM)=1
QUANT(NUM)=FIXPTV(I)
80 CONTINUE
C SEARCH DOTS AND QUANTITIES FOR EACH RUN
DO 90 I=1,NRUNS
IF(IY(I).NE.LINE) GO TO 90
NUM=NUM+1
IXC(NUM)=IX(I)
KORMT(NUM)=1
QUANT(NUM)=STAR
NUM=NUM+1
IXC(NUM)=IX(I)+1
KORMT(NUM)=2
ISUB=(I-1)*(NN+M+3)+K2+3
QUANT(NUM)=CPRT(ISUB)
90 CONTINUE
C FIND ASCENDING ORDER IN IXC OF POINTS.
IF(NUM) 95,95,100

```

```

95 WRITE(IOT,803)
    IF(LINE.GT.52) GO TO 145
    GO TO 45
100 DO 105 I=1,NUM
    LIST(I)=I
105 ORDR(I)=IXC(I)
    CALL ORDRFD(ORDR,LIST,NUM)
C PUT QUANT IN ORDR READY TO BE PRINTED OUT
    DO 110 I=1,NUM
        K22=K2-M
        QUANT(NUM-2)=CHEM(K22,1)
        QUANT(NUM-1)=CHEM(K22,2)
        QUANT(NUM)=CHEM(K22,3)
        GO TO 60
55 QUANT(NUM-2)=BLANK
    KL=LIST(I)
    J=NUM-I+1
110 ORDR(J)=QUANT(KL)
C CONSTRUCT FORMAT STATEMENT CORRESPONDING TO ITEMS ON THE CURRENT LINE
    LAST=0
    NTOT=0
    KF=1
    DO 135 KQ=1,NUM
        J=NUM-KQ+1
        KI=LIST(J)
        KIP=IXC(KI)-LAST-1
        IF(KIP) 130,130,115
115 L1=KIP/100
    L2=(KIP-L1*100)/10
    L3=(KIP-L1*100-L2*10)
    IF(L1.EQ.0) GO TO 120
    CH=DIC(21)
    GO TO 125
120 CH=DIC(1)
125 CT=DIC(L2+11)
    CU=DIC(L3+1)
    SKIP=OR(OR(FFOR,CH),OR(CT,CU))
    LAST=LAST+KIP
    IF(LAST.GE.119) GO TO 140
    KF=KF+1
    VFOR(KF)=SKIP
130 K1=KORMT(KI)
    LAST=LAST+NCHAR(K1)
    IF(LAST.GE.119) GO TO 140
    KF=KF+1
    VFOR(KF)=OUT(K1)
    NTOT=NTOT+1
135 CONTINUE
140 KF=KF+1
    VFOR(KF)=VLAST
    NUM=NTOT
C PRINT OUT TRIANGULAR DIAGRAM
    WRITE(IOT,VFOR) (ORDR(I),I=1,NUM)
    IF(LINE.LE.52) GO TO 45
145 IF(TX.LE.1.0) GO TO 150
    TX2=10./TX
    WRITE(IOT,804) ORGC,ORGH,TX2
C IF ALL DIAGRAMS ARE PRINTED OUT BOTH FOR ELEMENTS AND COMPOUNDS,
C RETURN. OTHERWISE PROCEED TO NEXT DIAGRAM
150 IF(K2.LT.(M+NN)) GO TO 20
    RETURN
C
C FORMAT SPECIFICATIONS
C
800 FORMAT(1H112A6,15X,5H PAGE,I4)
801 FORMAT(1H04H AT F5.1,9H ATM AND F7.2,7H KELVIN)
802 FORMAT(1H04H AT E8.2,9H ATM AND F7.2,7H KELVIN)
803 FORMAT(1X)
804 FORMAT(8H ORIGIN ,F7.4,12H PER CENT C ,F7.4,30H PER CENT H      SC
1ALE 1 INCH = ,F6.4, 9H PER CENT)
    END

```

```

C A DUMMY PROGRAM TO REPLACE TRIPRT IN CASE DIAGRAM IS NOT DESIRED
SUBROUTINE TRIPRT
RETURN
END

```

```

C BLOCK DATA STATEMENT TO PROVIDE A TABLE OF NAMES OF ELEMENTS
BLOCK DATA
COMMON /BLK2/TITLE(12),GF(20),TT(3),XX(15),AF(50),AELE(50),
1ELEMTS(15)
DATA (XX(I),I=1,15)/2H C,2H H,2H N,2H O,2H S,2H P,2HCL,2HBR,2H I,
12H K,2HCA,2HMG,2HCU,2HFE,2HSI/
END

```

#### LISTING OF SAMPLE DATA DECK

\$DATA					
C, H, O SYSTEM,	10ATM.,	1000K AND 1 ATM.,	500K	11/15/66	
•000000001	0.0003	•000000001	30	6	0.001 1.0
500.0	700.0	1000.0			
METHANE	-7.84	-3.05	4.61	C 1	H 4
H2	0.00	0.00	0.00	H 2	
O2	0.00	0.00	0.00	O 2	
WATER	-52.36	-49.92	-46.04	H 2	O 1
CO	-37.18	-41.53	-47.94	C 1	O 1
CO2	-94.39	-94.50	-94.61	C 1	O 2
BENZENE	39.24	48.21	62.27	C 6	H 6
NAPHTHALENE	68.72	81.17	99.85	C10	H 8
ASPHALT	160.68	183.96	218.88	C22	H12
ETHYLENE	19.25	22.68	28.25	C 2	H 4
			00	11	
ETHANE	1.17	10.90	26.13	C 2	H 6
METHANOL	-32.05	-25.14	-14.85	C 1	H 4 O 1
			00	00	
O2	•455	WATER		•01	
CO2	•02				
H2	•0008	WATER		•1246	
CO2	•1877	METHANE		•0123	
CO2	•1	METHANE		•113	
BENZENE	•0002	ASPHALT		•0039	
H2	•0001	CO		•0004	
CO2	•0998	METHANE		•068	
BENZENE	•0005	ASPHALT		•0104	

1	2	3	4
10.0		1000.0	
1.0		500.0	

**Appendix I**  
**Thermodynamic Equilibrium**  
**in Planetary Atmospheres**

## APPENDIX I

### THERMODYNAMIC EQUILIBRIA IN PLANETARY ATMOSPHERES

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Margaret O. Dayhoff,<sup>†</sup> and Carl Sagan<sup>II</sup>

#### Abstract

The thermodynamic equilibrium compositions of all possible combinations of the elements C, H, O, and N at reasonable average pressures and temperatures have been calculated for the atmospheres of Earth, Venus, Mars, and Jupiter. All regions of the composition diagram consistent with the observed molecular abundances are located and discussed.

The constituents of the terrestrial atmosphere considered as a closed system are in approximate thermodynamic equilibrium in spite of the continual addition of trace compounds by biological activity, lightning, radiation, and vulcanism. Under some circumstances, the presence of atmospheric organic molecules far in excess of their thermodynamic equilibrium proportions can be an indication of indigenous biological activity.

The atmosphere of Venus seems likely to be in thermodynamic equilibrium. It then follows that the measured upper limits on the abundances of CH<sub>4</sub>, NH<sub>3</sub>, and CO are all inconsistent with the possibility of elemental carbon or hydrocarbons in contact with the atmosphere, either on the surface or as clouds. If the Cytherean atmosphere evolved from an original gas mixture much more reducing than the present, two processes must have occurred: the loss of hydrogen to space and the loss of O<sub>2</sub>, most probably by efficient reaction with a considerable layer of reduced surface materials. In addition, Venus must have begun its evolutionary history with a [C/O] abundance ratio  $\leq 0.5$ , a value consistent with several cosmic abundance estimates.

The evidence for Mars is not inconsistent with thermodynamic equilibrium. The computations do not indicate whether small quantities of free O<sub>2</sub> exist. The equilibrium abundances of all oxides of nitrogen are extremely low even if computed with a considerable excess of O<sub>2</sub>.

For Mars and Venus there are no molecular species with a large predicted equilibrium abundance and spectroscopically accessible absorption features which have not already been identified.

Under equilibrium conditions at low temperatures Jupiter also cannot contain significant amounts of any molecule not yet observed. However, at high temperatures such as would be produced by lightning discharges or in the

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Jovian thermosphere, simple hydrocarbons and cyanides, polycyclic aromatics, and a variety of nitrogen compounds would be expected. Some of these compounds are brightly colored, and it seems possible that such organic compounds contribute to the observed variable coloration of Jupiter.

## Introduction

The gross chemical composition of planetary atmospheres can be approximated to some degree as the thermodynamic equilibrium distribution of the constituent atoms. In the upper reaches of planetary atmospheres, where the optical depth at ultraviolet frequencies is small, relative molecular abundance may be dominated by photodissociation and recombination. In the lower portions of the atmospheres, which are shielded from photodissociating ultraviolet radiation, a closer approximation to thermodynamic equilibrium can be expected. Especially where surface temperatures are high or when catalysts such as water are present, there will be a strong tendency for the degradation of molecules to the lowest energy state. Even in the presence of special mechanisms which favor the production of specific compounds -- mechanisms such as ultraviolet radiation or lightning -- the thermodynamic equilibrium distribution of reaction products should be a useful first-order approximation. Since the equilibrium state is independent of particular reaction mechanisms and reaction rates, and since the computations of equilibrium states are quite straightforward, studies of thermodynamic equilibrium chemistry would appear prerequisite to considerations of nonequilibrium processes.

One of the earliest examples of a fruitful argument from thermodynamic equilibrium in planetary atmospheres was provided by Wildt (1937), who pointed out that the absence of detectable amounts of higher hydrocarbons, both saturated and unsaturated, in the atmospheres of the Jovian planets was an argument for the presence of a great excess of molecular hydrogen, a gas which had not been detected at that time. Further indirect evidence for the presence of low-mass constituents in the Jovian atmosphere was provided by observations of the occultation of  $\sigma$  Arietis, by Baum and Code (1953); but not until fairly recently were the quadrupole lines of  $H_2$  observed directly in the photographic infrared (Kiess, Corliss, and Kiess 1960). Urey (1959) has argued from the large abundance of carbon dioxide on Venus that substantial quantities of  $CH_4$ ,  $NH_3$ ,  $H_2$ ,  $N_2O$ , and other oxides of nitrogen would not be expected on that planet. A very low upper limit on the allowed abundance of oxides of nitrogen in the Martian atmosphere was set by Sagan, Hanst, and Young (1965) in a discussion of combined photochemical and thermodynamic equilibria. Wildt (1937) and Urey (1952), while performing thermodynamic equilibrium calculations in a planetary atmospheres context, stressed the possibility of significant departures from thermodynamic equilibrium.

Some more recent studies have suggested that thermodynamic equilibrium calculations may, under certain circumstances, be a useful approximation to reality. Thermodynamic equilibrium calculations by Dayhoff, Lippincott, and Eck (1964) for the relative abundances of a large number of compounds of biological interest have been performed under a wide variety of assumed conditions

of temperature, pressure, and elemental composition. These machine computations have revealed a possible mechanism for the abiological formation of polycyclic aromatic hydrocarbons (asphaltic tars) and have shown the existence of an oxidation threshold where free oxygen appears and at which all but the simplest organic compounds disappear. Studier, Hayatsu, and Anders (1965) have recently called attention to a remarkable agreement between the distribution of organic compounds observed in the carbonaceous chondrites, and that which was predicted from thermodynamic equilibrium calculations in the range of elemental abundances where asphaltic tars are expected. This success has encouraged us to extend thermodynamic equilibrium calculations to planetary atmospheres.

### Methods of Calculation

Our computational procedures have been described previously (see Chapter 2) following a well-known method (White, Johnson, and Dantzig 1958) which minimizes the free energy of the system, simultaneously satisfying the equilibrium constants of all possible reactions. The calculations were performed on an IBM 7094 computer.

At thermodynamic equilibrium, the distribution of molecular species is independent of the specific reaction pathways by which equilibrium is attained. The molecular balance depends upon the relative elemental abundances, pressure, temperature, and the standard free energies of formation of the compounds. All compounds present in significant concentrations must be included in order to arrive at the correct molecular distribution. Fortunately, there are only a small number of these major compounds; they are simple in structure and well known to chemists. For a real system to approach equilibrium, there need be only one reversible reaction pathway which leads from the major constituents to the other compounds.

In our computations on planetary atmospheres, we explored the entire range of possible relative atomic compositions using a large number of molecular species in order to locate any specific ranges of atomic abundances which would be simultaneously compatible with all the existing estimates of molecular abundances or their upper limits. The results are presented in ternary diagrams which cover all possible proportions of the elements C, H, and O. Compounds of nitrogen can also be represented as a projection on this diagram. The astronomical observation of a specific relative abundance for a given molecular species will, in general, define a line on the ternary diagram. An upper or lower concentration limit will exclude a certain area. The application of several such constraints may operate in a mutually inconsistent manner, so that no point on the diagram simultaneously satisfies all observations. In such a case, we would conclude that thermodynamic equilibrium is not attained in this atmosphere. On the other hand, if the application of several such constraints can be performed in a consistent manner, yielding a region of the ternary diagram simultaneously compatible with all constraints, we might tentatively conclude that the thermodynamic equilibrium is a useful first approximation to the atmosphere in question. Each point in the allowed region of the diagram would then correspond to a possible elemental composition in the

planetary atmosphere. The calculations would place some upper and lower limits on the allowable relative abundances of other possible constituents of the atmosphere.

### Observational Limitations

The initial conditions for these computations are based upon the results of astronomical spectroscopy. It is not a trivial matter to derive relative abundances from such observations. The conversion of equivalent widths to absolute abundances requires careful laboratory calibrations. Intercomparisons of abundances derived for the same molecule at different wavelengths must allow for the possibility that the effective reflecting atmospheric level is a function of wavelength. Existing observational discrepancies on, for example, the abundance of water vapor in the atmosphere of Venus (see, e. g., the discussion by Sagan and Kellogg 1963) underscore the uncertainties of such reductions. Intercomparisons of the relative abundances of different molecular species is even more uncertain. Determinations of absolute abundances is complicated by the possibility of multiple scattering (see Chamberlain 1962, 1965). Observations of very weak lines of a given molecular species may refer to substantial depths in the planetary atmosphere, where ultraviolet photodissociation is not a dominant process. Observations of strong lines may refer to high altitudes alone, where the relative distribution of molecular species may be far from that predicted by thermodynamic equilibrium. However, the species must be derivable from some compounds present extensively in the atmosphere.

Bearing these cautions in mind, we now proceed to a discussion of thermodynamic equilibrium in the atmospheres of the planets Earth, Venus, Mars, and Jupiter. In general, the conclusions we will draw will not be sensitively dependent on the exact values of the adopted mixing ratios of minor constituents; and variations in these mixing ratios even by several orders of magnitude will leave most of the results unchanged. Thus, despite the uncertainties in the observational material, it will nevertheless be possible to draw conclusions of some significance.

### The Earth

As a test of our computation procedures, we first consider thermodynamic equilibrium in the terrestrial atmosphere assuming this as a closed system. In addition to its major components, the atmosphere of the Earth contains a variety of compounds of diverse origins: methane and smaller amounts of other hydrocarbons from natural gas, petroleum, and asphalt; sulfur dioxide, hydrogen sulfide, carbon monoxide, and nitrogen oxides from vulcanism; terpenes and other volatile organics from vegetation; methane,  $N_2O$ , and hydrogen sulfide from the metabolic processes of microorganisms; ozone and nitrogen oxides from lightning and solar radiation, etc. Table 1 shows the amounts of some of these compounds which have been detected in the open air.

TABLE 1  
ADOPTED CHEMICAL COMPOSITION AND PHYSICAL  
PARAMETERS OF THE TERRESTRIAL ATMOSPHERE  
(VOLUME MIXING RATIOS ARE DISPLAYED)

O <sub>2</sub>	0.2095
O <sub>3</sub>	10 <sup>-8</sup> to 10 <sup>-7</sup>
H <sub>2</sub>	5 X 10 <sup>-7</sup>
H <sub>2</sub> O	1 X 10 <sup>-3</sup> to 2.8 X 10 <sup>-2</sup>
N <sub>2</sub>	0.7808
NO <sub>2</sub>	5 X 10 <sup>-10</sup> to 2 X 10 <sup>-8</sup>
N <sub>2</sub> O	5 X 10 <sup>-7</sup>
NH <sub>3</sub>	1.7 X 10 <sup>-8</sup>
SO <sub>2</sub>	1 X 10 <sup>-6</sup>
CO <sub>2</sub>	3.30 X 10 <sup>-4</sup>
CH <sub>4</sub>	1.5 X 10 <sup>-6</sup>
A	1 X 10 <sup>-2</sup>
He	5.2 X 10 <sup>-6</sup>
Ne	1.8 X 10 <sup>-5</sup>
Pressure	1.0 atm.
Temperature	280°K

(References: Allen 1963; Hutchinson 1954)

TABLE 2  
THERMODYNAMIC EQUILIBRIUM COMPOSITION OF THE  
TERRESTRIAL ATMOSPHERE, COMPUTED FROM THE  
TOTAL ELEMENTAL COMPOSITION OF TABLE 1\*

N <sub>2</sub>	0.78	H <sub>2</sub> S	0
O <sub>2</sub>	0.21	CO	0
A	0.01	H <sub>2</sub>	0
H <sub>2</sub> O	1.0 X 10 <sup>-3</sup>	CS <sub>2</sub>	0
CO <sub>2</sub>	3.3 X 10 <sup>-4</sup>	CH <sub>4</sub>	0
SO <sub>3</sub>	1 X 10 <sup>-6</sup>	CH <sub>3</sub> SH	0
HNO <sub>3</sub>	5 X 10 <sup>-10</sup>	COS	0
NO <sub>2</sub>	7 X 10 <sup>-11</sup>	Benzene	0
NO	3 X 10 <sup>-17</sup>	Formic acid	0
H <sub>2</sub> SO <sub>4</sub>	4 X 10 <sup>-18</sup>	HCN	0
SO <sub>2</sub>	8 X 10 <sup>-20</sup>	NH <sub>3</sub>	0
N <sub>2</sub> O	2 X 10 <sup>-20</sup>	Formaldehyde	0
Ozone	6 X 10 <sup>-32</sup>	Methanol	0

\*A mixing ratio of zero is an abbreviation for  
a value <10<sup>-35</sup>.

We have calculated the balance of compounds for every combination of C, H, O, and N at 1 atm. and 280°K. The only equilibrium consistent with the observed major constituents in Table 1 is shown in Table 2. Such a point where major constituents in the terrestrial atmosphere are completely compatible with thermodynamic equilibrium need not necessarily exist. For example, large quantities of CO, natural gas, or H<sub>2</sub>S might be admixed. All of these would decompose at thermodynamic equilibrium in the presence of excess oxygen. Any carbon in the atmosphere would occur as CO<sub>2</sub>, and any sulfur as SO<sub>3</sub>. Since there is no reason to think that less oxidized materials are presently accumulating in the atmosphere, they must be in approximate dynamic equilibrium, being removed or destroyed as fast as they are being added. That is, even at the prevailing low temperatures there is a definite tendency for the Earth's atmosphere to approach thermodynamic equilibrium. Such reactions are no doubt catalyzed by solar radiation and by dust particles and droplets suspended in the air. This constitutes a specific example of our general contention that, even in the presence of special mechanisms which favor the production of certain specific compounds, the overall tendency will be for a planetary atmosphere to approach thermodynamic equilibrium. If the major components of the atmosphere were methane, hydrogen, water, and nitrogen (or ammonia) instead of the present composition, the products of the radiation-coupled reactions would be different, but the overall trend to thermodynamic equilibrium would still be present. If the crust and oceans were also included, equilibrium would not obtain. However, the transfer between phases is slow relative to reactions within the gas phase. It is not obvious at what relative rates unstable prebiological compounds such as amino acids would be produced by nonequilibrium processes and degraded by the environment and by their interaction with each other.

The observation of complex, very energetic compounds such as terpenes in the contemporary atmosphere of the Earth would lead an extraterrestrial observer to suspect the existence of life here. The lack of any obvious simple mechanism to form terpenes, either by thermodynamic equilibrium at some plausible combination of elemental composition, temperature, and pressure, or by photochemical reactions or other physical processes, would indicate the presence of biological activity on the Earth -- even in the absence of any other signs of life. Simpler highly reduced substances also exist far in excess of their thermodynamic equilibrium proportions in the oxidizing terrestrial atmosphere -- e.g., CH<sub>4</sub> (compare Tables 1 and 2). Such materials would therefore also be a possible test for indigenous biology; but since other plausible origins could be imagined for them -- e.g., the decomposition of prebiologically synthesized polycyclic aromatics -- the presence of such molecules would be inconclusive for biology. In fact, methane has such a high abundance in the terrestrial atmosphere only because of the metabolic activities of micro-organisms (see, e.g., Hutchinson 1954).

## Venus

The observational constraints on the atmospheric composition of Venus are given in Table 3, constructed from the references there given. Some comments should be made on the values adopted for  $[CO_2]^*$ ,  $[H_2O]$ , and  $[CO]$ . The 5% volume mixing ratio of carbon dioxide adopted in our analysis is a fairly conventional one, derived from Spinrad's (1962a) observations, and dependent upon the assumption that the near infrared  $CO_2$  bands are formed by single scattering. Chamberlain (1965) has recently shown that the introduction of multiple scattering might reduce the  $CO_2$  mixing ratio by as much as an order of magnitude. The precise reduction factor is at the present time unknown. However, similar correction factors for multiple scattering will be applicable to all other abundances and abundance upper limits of Table 3, and relative abundances of all minor constituents should be approximately those of Table 3, whether single or multiple scattering is assumed. The relative abundance of the major atmospheric constituents -- probably  $N_2$ , with some admixture of noble gases -- would then vary from 95% to larger values. Such variations have no significant effects on our conclusions.

Reported observations of water vapor in the spectrum of Venus have been made by Dollfus (1964) and by Bottema, Plummer, and Strong (1964). The derived values of the water vapor mixing ratio depend on the scattering mechanism and the total atmospheric pressure at the effective level of band formation. The range of derived mixing ratio values shown in Table 3 is consistent (Sagan and Kellogg 1963, Chamberlain 1965) with a previous upper abundance limit on water vapor established by Spinrad (1962b). However, the water vapor which is observed by infrared spectroscopy may be primarily in the region of the clouds. Since there is now fairly convincing evidence that the clouds are condensed water (Bottema, Plummer, Strong, and Zander 1964, Sagan and Pollack 1966a), it is in general invalid to assume that the water vapor mixing ratio in the vicinity of the clouds applies to the lower Cytherean atmosphere. The amount of condensed water in the clouds required to explain the near infrared reflection spectrum of Bottema, Plummer, Strong, and Zander (1964), and also to explain the millimeter attenuation of the surface thermal microwave emission, is  $1 \text{ gm cm}^{-2}$  or less; convective atmospheres which can maintain such clouds at the observed pressures and temperatures must have volume mixing ratios of water vapor in their lower reaches of a few times  $10^{-4}$  (Sagan and Pollack 1966b). The water vapor mixing ratio may therefore range from a few times  $10^{-6}$  in the vicinity of the clouds and above, to a few times  $10^{-4}$  near the Cytherean surface.

The quantities of carbon monoxide in the spectrum of Venus observed by Moroz (1965), if related to a 1 atm. pressure level near the cloudtops, give a volume mixing ratio  $\sim 10^{-6}$ . However, CO is a principal carbon dioxide photodissociation product, and amounts of carbon monoxide almost comparable to those reported by Moroz may arise from photodissociation (Moroz 1965, Shimizu 1963).

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\* In the following discussion square brackets denote volume mixing ratios.

If the observed carbon monoxide abundance is significantly in excess of that expected from photochemical equilibrium, then a CO mixing ratio of  $10^{-6}$  may be extended down to the lower Cytherean atmosphere. If, on the other hand, the observed carbon monoxide is due principally to photochemical processes, then the carbon monoxide abundance in the lower Cytherean atmosphere will be substantially less.

We adopt a Venus surface temperature of 700°K, and a surface pressure of 50 atm. (Sagan 1962, Pollack and Sagan 1965). Moderately large departures from these values will not alter our conclusions significantly. In particular, the calculations performed at such pressures and temperatures should, because of the relative pressure and temperature insensitivity of the reaction thresholds and because of atmospheric convection, be applicable to a major fraction of the total mass of the Cytherean atmosphere.

A ternary diagram showing all possible combinations of the elements C, H, and O is presented in Figure 1. The corners of the triangle represent pure

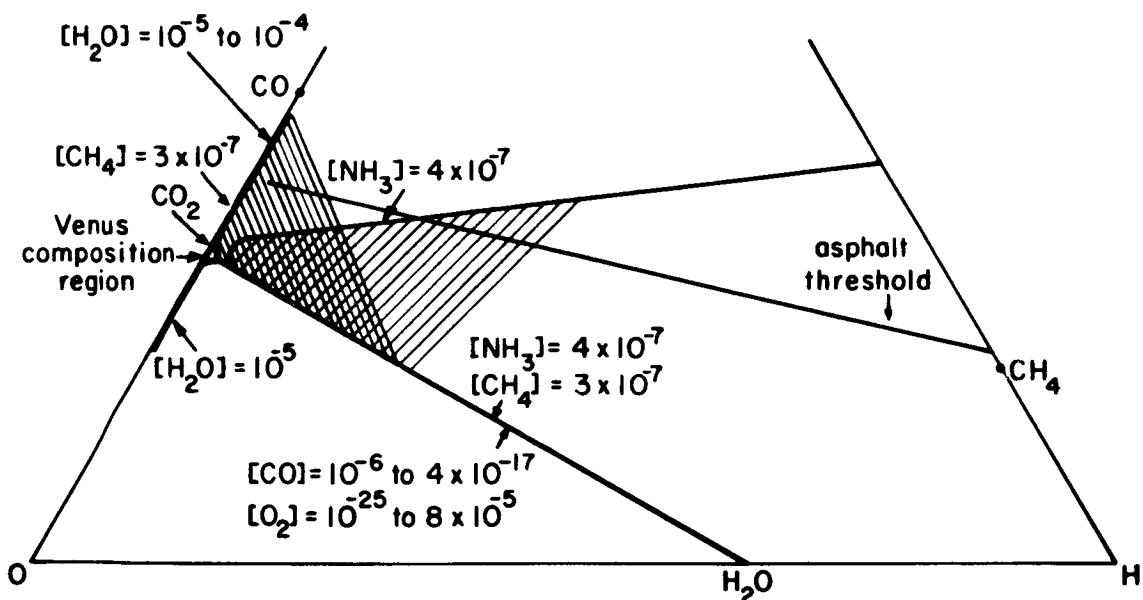


Figure 1. C-H-O ternary diagram for the Cytherean atmosphere. The shaded regions are excluded at thermodynamic equilibrium by the observational upper limits on  $[CH_4]$  and  $[NH_3]$ . For clarity the shading has not been extended through the entire excluded region. The adopted values of  $[H_2O]$  and the observed upper limits on  $[CO]$  and  $[O_2]$  are denoted by lines.

carbon, pure hydrogen, and pure oxygen. The positions of pure carbon dioxide and pure water are also indicated. The line connecting the  $\text{CO}_2$  and  $\text{H}_2\text{O}$  points is an oxidation threshold, which divides the diagram into an upper, reducing, portion in which sizable numbers of different species of organic molecules may be expected at thermodynamic equilibrium, and a lower, oxidizing, portion, in which such molecules are unstable, and in which free oxygen exists. Also indicated in Figure 1 is the asphaltic tar threshold. Above this line, polycyclic aromatic hydrocarbons occur at thermodynamic equilibrium (in the absence of a mechanism to form graphite); below it, they are excluded. Since graphite is not observed in heat-catalyzed reactions involving temperatures of 700°K (Studier, Hayatsu, and Anders 1966) and in quenched plasmas (Eck, Lippincott, Dayhoff, and Pratt 1966), the computations have been extended past the line of graphite precipitation.

The ammonia upper abundance limit of  $4 \times 10^{-7}$  restricts the atmosphere at thermodynamic equilibrium to the region below the line marked  $\text{NH}_3$  in Figure 1. This line lies in the reducing region of the diagram, slightly above the oxidation threshold, and curves away from the carbon dioxide point, as illustrated. This one spectroscopic upper limit therefore excludes most of the reducing portion of the ternary diagram. The concentration of ammonia varies so rapidly in the region of the illustrated line that the width of this line represents several orders of magnitude in concentration -- an example of the insensitivity of these calculations to exact relative abundances.

We next consider the upper abundance limit on methane. This concentration yields a curve which closely follows the C-O edge until the  $\text{CO}_2$  point is reached, whereupon it swings away and follows the oxidation threshold. The  $\text{CH}_4$  curve is even more constraining than the  $\text{NH}_3$  curve, and excludes almost the entire reducing portion of the diagram.

We now consider the constraints imposed by the water vapor mixing ratio. Figure 1 shows a line for  $[\text{H}_2\text{O}] = 10^{-5}$ , which, in the oxidizing region of the diagram, lies very close to the C-O edge. The curves for mixing ratios an order of magnitude larger would lie very close to the curve shown. Thus, the searches for methane, ammonia, and water have restricted the equilibrium chemistry of the Cytherean atmosphere to a very narrow region of the ternary diagram, hugging the C-O edge throughout the oxidizing region, and extending very slightly into the reducing region.

In Figure 2, where the Venus ternary diagram has been magnified 100 times, the line corresponding to a carbon monoxide volume mixing ratio of  $[\text{CO}] = 10^{-6}$  is indicated. Since part of the observed carbon monoxide may be due to  $\text{CO}_2$  photodissociation, the fraction of carbon monoxide relevant for thermodynamic equilibrium calculations will be somewhat less than  $10^{-6}$ . The observations therefore further restrict the ternary diagram to the area below the line  $[\text{CO}] = 10^{-6}$ . We see that this line closely parallels the oxidation threshold. As with the  $\text{NH}_3$  and  $\text{CH}_4$  lines, the width of the  $[\text{CO}] = 10^{-6}$  line actually corresponds to many orders of magnitude in the mixing ratio. The lower side of this line corresponds to the oxygen upper abundance limit,  $8 \times 10^{-5}$ . If observations can establish any detectable amount ( $>10^{-16}$ ) of CO in the lower atmosphere, the amount of  $\text{O}_2$  must be extremely small. Conversely, if

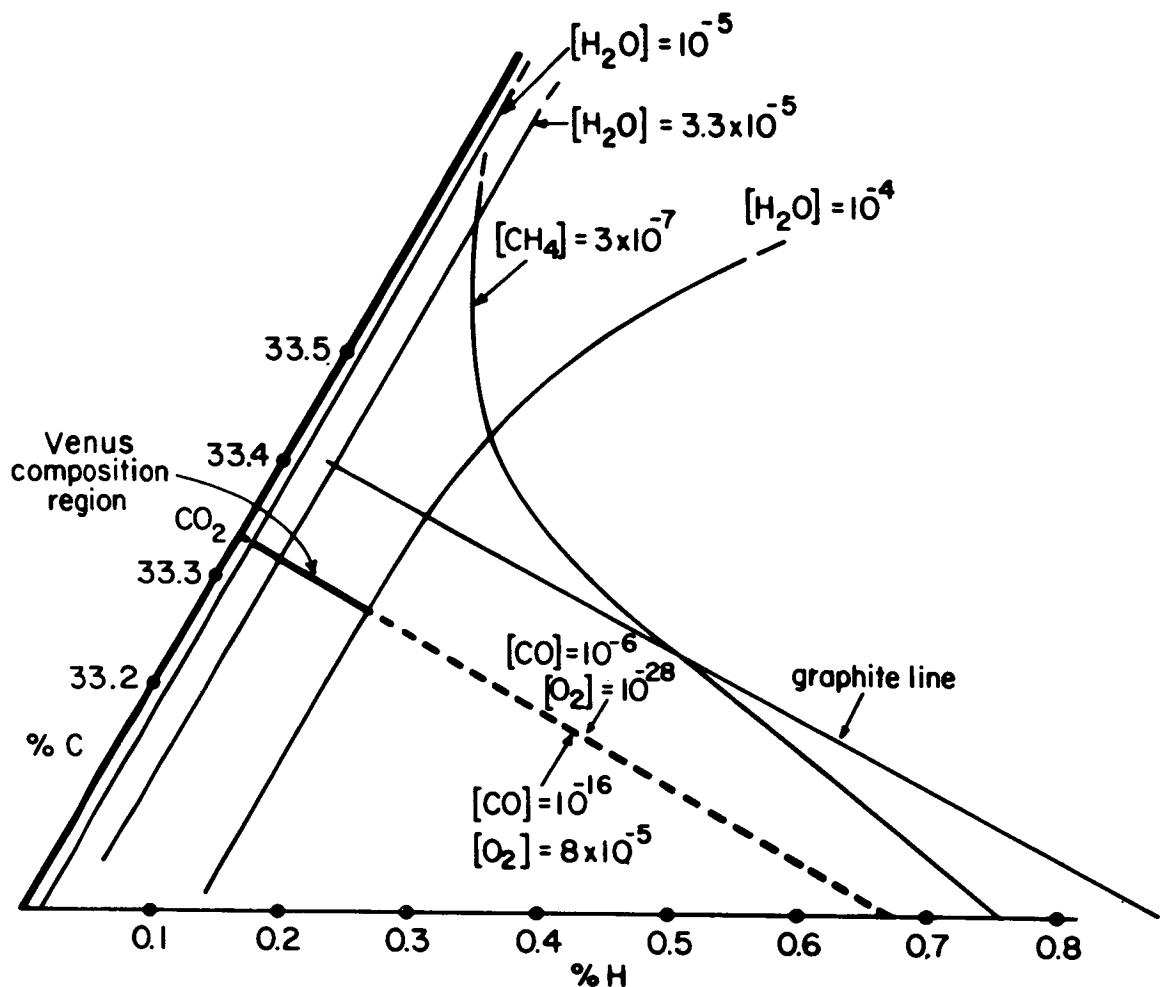


Figure 2. C-H-O ternary diagram of Fig. 1, here enlarged one hundredfold.

$[O_2] \geq 8 \times 10^{-5}$ , then  $[CO] \leq 4 \times 10^{-17}$ . At any rate the upper limits on Cytherean [CO] and  $[O_2]$  restrict the thermodynamic equilibrium composition to the thickness of the thick slant line in Figures 1 and 2.

In Figure 2 is displayed a line above which a solid phase of graphite might form. The composition of the atmosphere is clearly incompatible with solid carbon in equilibrium in the atmosphere or on the surface. Similarly, any equilibrium accumulation of polycyclic aromatics, or any other hydrocarbons, is forbidden, a conclusion reached for a much smaller array of compounds by Mueller (1964). The asphalt threshold seen in Figure 1 lies well into the region excluded by the unsuccessful searches for  $CH_4$  and  $NH_3$ . This conclusion is separately confirmed by the CO upper abundance limits, and is independent

of the quantity of water present. This exclusion of hydrocarbons is relevant to some models of the Venus atmosphere which invoke hydrocarbon clouds (Kaplan 1963). The absence of polycyclic aromatic hydrocarbons from the surface is consistent both with passive observations of the microwave phase effect and with active radar observations of Venus (Pollack and Sagan, 1965).

Table 4 shows the chemical composition of the atmosphere of Venus, at two extremes of CO and O<sub>2</sub> concentration, predicted from thermodynamic equilibrium. If the measured value of CO depends entirely on photodissociation, then there may be as much as [O<sub>2</sub>] = 8 X 10<sup>-5</sup>. We emphasize again that any error in the relative abundance of nitrogen would cause negligible deviation in the relative abundance of carbon compounds, and indeed, would have very little effect on the calculated ammonia abundance. A smaller amount of nitrogen would only make the ammonia concentration a less severe restriction on the actual composition (cf. Figure 1). The constituents shown at the bottom of the table would be formed if 0.0001% sulfur were added to the atmosphere.

Formaldehyde was once suspected in the atmosphere of Venus (Wildt, 1940) but at thermodynamic equilibrium with the detected amounts of water and the observational upper limit on methane, the concentration of formaldehyde would be negligible. Non-equilibrium reactions in simulated Cytherean atmospheres are known, however, to produce formaldehyde (Sagan and Miller, 1960).

We now explore some other consequences of the foregoing abundances. Possible atmospheric compositions are limited to a segment of the [CO] = 10<sup>-6</sup> curve near [H<sub>2</sub>O] = 10<sup>-4</sup>, as shown in Figure 2. The composition of Venus is then specified by a segment of one thick line in the ternary diagram, near the CO<sub>2</sub> composition point, and slightly on the reducing side of the oxidation threshold. This conclusion is consistent with all abundance determinations and upper limits. The fact that none of the observations are mutually inconsistent suggests that the atmosphere of Venus is, on the whole, close to that predicted by thermodynamic equilibrium.

It should be emphasized that the finding that the predicted thermodynamic equilibrium is consistent with the available observations is not trivial. Whatever the given molecular species used to define a particular atomic composition of the atmosphere, the computed equilibrium molecular proportions would be the same. Neither can one predict *a priori* which of the major compounds would be present, given a particular elemental composition. The proportions 1C: 2H: 20 give the empirical formula of formic acid, but this compound would be only a minor component of the equilibrium mixture. The same proportions apply to an equimolar mixture of CO and H<sub>2</sub>O. However, a gas composed of these two compounds is not the correct answer, either. The equilibrium result is a mixture of H<sub>2</sub>O, CH<sub>4</sub>, and CO<sub>2</sub> -- unless the computation had been for a higher temperature, in which case there would also have been appreciable amounts of CO and H<sub>2</sub>.

A disagreement between predicted and observed results can occur in two ways. First, a definite observed species may be unobtainable at equilibrium. If 1 percent of HCN had also been observed on Venus, we would have found no C:H:O proportions for which this large amount would be predicted. Such an

TABLE 3

ADOPTED CHEMICAL COMPOSITION OF THE  
CY THEREAN ATMOSPHERE  
(VOLUME MIXING RATIOS ARE DISPLAYED)

$O_2$	$<8 \times 10^{-5}$	$CO_2$	$\sim 5 \times 10^{-2}$
$H_2O$	$1 \times 10^{-6}$ to $1 \times 10^{-4}$	$CO$	$<1 \times 10^{-6}$
$N_2$	~0.95	$CH_4$	$<3 \times 10^{-7}$
$NO_2$	$<1 \times 10^{-6}$	$C_2H_4$	$<2 \times 10^{-7}$
$N_2O$	$<4 \times 10^{-7}$	$C_2H_6$	$<1 \times 10^{-7}$
$NH_3$	$<4 \times 10^{-7}$	$HCHO$	$<3 \times 10^{-8}$
Pressure	~50 atm	Temperature	700°K

(References: Kuiper 1952; Spinrad 1962a, 1962b; Spinrad and Richardson 1965; Bottema, Plummer, and Strong 1964; Dollfus 1964; Sagan and Pollack 1966b)

TABLE 4

THERMODYNAMIC EQUILIBRIUM COMPOSITION OF  
THE CY THEREAN ATMOSPHERE, COMPUTED  
FROM TOTAL ELEMENTAL COMPOSITION OF TABLE 2\*

Compound	Oxidizing Limit	Reducing Limit
$O_2$	$8 \times 10^{-5}$	$4 \times 10^{-26}$
$CO$	$2 \times 10^{-17}$	$1 \times 10^{-6}$
$CO_2$	$5 \times 10^{-2}$	$5 \times 10^{-2}$
$H_2O$	$1 \times 10^{-5}$	$1 \times 10^{-5}$
$N_2$	0.95	0.95
$H_2$	$4 \times 10^{-20}$	$2 \times 10^{-9}$
$NH_3$	$4 \times 10^{-30}$	$4 \times 10^{-14}$
$HCN$	0	$2 \times 10^{-18}$
$NO$	$7 \times 10^{-9}$	$2 \times 10^{-19}$
$NO_2$	$10^{-9}$	$4 \times 10^{-31}$
$N_2O$	$6 \times 10^{-12}$	$1 \times 10^{-22}$
$HNO_3$	$1 \times 10^{-14}$	0
$O_3$	$3 \times 10^{-20}$	0
Methane	0	$8 \times 10^{-21}$
Ethane	0	0
Formic Acid	$5 \times 10^{-26}$	$2 \times 10^{-15}$
Formaldehyde	0	$3 \times 10^{-19}$
Methanol	0	$9 \times 10^{-26}$
Acetic Acid	0	$6 \times 10^{-28}$
Methyl Amine	0	$6 \times 10^{-33}$
Acetylene	0	$5 \times 10^{-34}$
Benzene	0	0
Asphalt	0	0
$SO_2$	$6 \times 10^{-8}$	$1 \times 10^{-6}$
$SO_3$	$1 \times 10^{-6}$	$4 \times 10^{-16}$
$COS$	0	$1 \times 10^{-7}$
$H_2S$	0	$5 \times 10^{-9}$
$CH_3SH$	0	$5 \times 10^{-26}$
$H_2SO_4$	$5 \times 10^{-17}$	$2 \times 10^{-26}$

\*Two extreme systems,  $[CO] = 10^{-6}$ ,  $[O_2] = 4 \times 10^{-26}$  and  $[CO] = 2 \times 10^{-17}$ ,  $[O_2] = 8 \times 10^{-5}$ , are shown. The hypothesized sulfur mixing ratio of  $10^{-6}$  has a negligible effect except on compounds containing sulfur.

observation would have been inconsistent with the hypothesis of thermodynamic equilibrium on Venus.

Secondly, all systems consistent with the observed concentrations could also contain observable quantities of compounds which were not in fact observed. Such inconsistencies were sought, but not found. We therefore conclude that the results are consistent with general thermodynamic equilibrium on Venus; only a very limited fraction of the atmosphere is being produced by such special processes as discussed for the earth's atmosphere.

### Evolution of the Atmosphere of Venus

In this case some remarks can be made on the original composition and subsequent evolution of the Cytherean atmosphere. From cosmic abundance considerations, it is clear that the atmosphere must originally have had a composition putting it in the extreme right-hand corner of the ternary diagram (see Figure 3), if the atmosphere was originally derived from a solar nebula. If it was derived from vulcanism, the composition would have been somewhere in the middle of the reducing region, and the following considerations would apply just as well. The chemical evolution of the atmosphere occurs initially through the escape of atomic hydrogen from the Cytherean exosphere. Escape of significant quantities of carbon or oxygen from Venus during geological time seems quite unlikely (see, e.g., Sagan, 1966). Any differential escape is correspondingly unlikely. The track along which the atmospheric composition of Venus evolves depends then on the initial carbon-to-oxygen abundance ratio. The cosmic [C/O] abundance ratio has been assigned a value of 0.20 by Suess and Urey (1956), while Cameron (1959) has suggested a value of 0.44 and more recently (1963), 0.67. For a ratio of 0.20 or 0.44, the evolution would proceed along the lines ending at  $\alpha$  or  $\beta$  (Figure 3), in a region where free oxygen exists. For an initial [C/O] ratio of 0.67, the evolutionary track ends at  $\gamma$ , in the reducing portion of the diagram. The actual present atmosphere of Venus appears to have a [C/O] ratio that differs from that of  $\text{CO}_2$  by an amount  $10^{-5}$  or less. If the initial atmosphere had a [C/O] ratio anywhere between 0.2 and 0.7, the probability that the present ratio would be as close to  $\text{CO}_2$  as it appears to be, through no other process but the loss of hydrogen, would then be about  $4 \times 10^{-5}$ . This seems quite unlikely. However, if oxygen were also depleted from the atmosphere, then over a wide range of initial [C/O] ratios the atmosphere would finally settle at the  $\text{CO}_2$  point. Since it seems unlikely that oxygen has escaped from Venus, the depletion of atmospheric oxygen must be attributed to chemical reactions, and the surface material of Venus, initially reducing, must now be partially oxidized to a considerable depth. An independent argument for the presence of extensive oxygen sinks on the surface of Venus has been offered by Sagan (1966), in an attempt to explain the differential abundance of water on Venus and on Earth by differential rates of water photodissociation.

Typical evolutionary tracks would then have resembled those illustrated by the arrows in Figure 3. Due to loss of hydrogen, the atmosphere evolves away from the hydrogen corner of the ternary diagram until it intersects the oxidation threshold. As soon as free oxygen is produced, it combines with

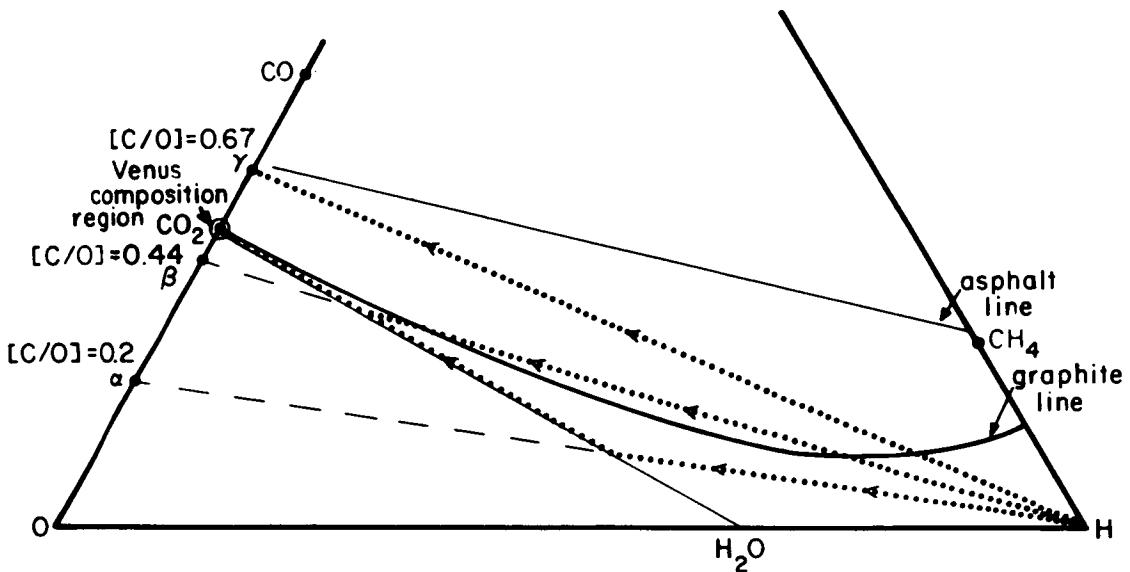


Figure 3. Evolution of the atmosphere of Venus. Initial conditions assumed include a large excess of  $H_2$ , and three  $[C/O]$  abundance ratios. Loss of hydrogen alone causes evolution along the tracks  $H-\alpha$ ,  $H-\beta$ , and  $H-\gamma$ . Additional loss of oxygen would tend to deflect the lower two evolutionary tracks along the oxidation threshold, the line  $CO_2 - H_2O$ . Tracks with initial  $[C/O] > 0.5$  must lose carbon to arrive at the present composition; but the precipitation of graphite or polycyclic aromatics would not lead to the contemporary value of  $[C/O]$ .

surface material and the evolutionary track turns abruptly upward, following the oxidation threshold toward the  $CO_2$  point.

If the initial  $[C/O]$  ratio were 0.44, the initial evolutionary track due to the loss of hydrogen would twice intersect the graphite threshold (cf. Figure 3). There would then be an interlude in the evolutionary history of Venus in which graphite might be present. However, the activation energy for

the formation of graphite is so great that it would very likely never precipitate directly. If it did, it would react and disappear as the system lost more hydrogen. Such a track would follow the line marked H- $\beta$  until it intersected the oxidation threshold, whereupon it would turn and proceed toward the CO<sub>2</sub> point.

If the initial [C/O] ratio were 0.67, the evolutionary track would follow the line marked H- $\gamma$  in Figure 3. This line intersects the graphite threshold once, and never crosses the oxidation threshold. The atmosphere would then always remain in the reducing portion of the diagram. In order to end at the CO<sub>2</sub> point, some mechanism must exist for the removal of carbon from the atmosphere or the addition of oxygen to it. The asphalt threshold is not intersected, so no formation of polycyclic aromatics would be expected. If the removal of carbon from the atmosphere were possible -- for example by the precipitation of graphite or organic material -- the atmosphere would then evolve along the graphite line. As the C-O line was approached, any such exposed, precipitated graphite would undergo equilibrium reactions with the atmosphere and disappear. The composition would end significantly above the actual composition point, where the CO concentration would be 10<sup>-3</sup>, in conflict with the spectroscopic observations. While the outgassing of water, photo-dissociation, and hydrogen escape could conceivably increase the O<sub>2</sub> abundance over a surface which was not highly reducing, the addition of precisely enough O<sub>2</sub> to bring the atmosphere to its present unique composition very close to the CO<sub>2</sub> point is highly implausible. It is interesting to note that if the temperature of Venus were much lower, for example, 500°K, graphite could exist in equilibrium with the observed atmosphere, if a mechanism were available for its formation. However, no complex organic compounds would be stable even under these conditions.

Thus, it is probable that Venus began its evolutionary history with a [C/O] abundance ratio  $\leq 0.5$  and that its evolutionary track in the ternary diagram was directed towards the CO<sub>2</sub> point by the simultaneous loss of hydrogen to space and oxygen to the surface.

### Mars

Because of the low temperature and relative ultraviolet transparency of the Martian atmosphere, the applicability of thermodynamic equilibrium calculations should be more limited than in the case of Venus. The character of the equilibrium state is nevertheless of interest. A surface temperature of 240°K and a surface pressure of 50 mb was assumed for the Martian atmosphere (Kaplan, Munch, and Spinrad, 1964; Hanst and Swan, 1965). Our remarks on the insensitivity of the calculations to the precise values of pressures and temperatures apply again to this case and a surface pressure of 10 mb would not appreciably alter the results. The observational constraints on the atmospheric composition are shown in Table 5. The atmosphere is assumed to be approximately 90% molecular nitrogen and noble gases. The remainder of the atmosphere is expected to be compounds of carbon, oxygen, nitrogen, and hydrogen. The anticipated CO<sub>2</sub> mixing ratio is not known at the present time. Its

value is tied closely to the value of the absolute surface pressure (Kaplan, Munch, and Spinrad, 1964; Hanst and Swan, 1965; Chamberlain and Hunten, 1965). The values of Table 5 correspond to the range of suggested values at the time of writing. As in the case of Venus, the absolute value of the  $\text{CO}_2$  mixing ratio is not critical in computations of the relative values of the mixing ratios of minor constituents.

The ammonia upper abundance limit excludes the highly reducing portion of the ternary diagram, as shown in Figure 4. The upper limit on the methane

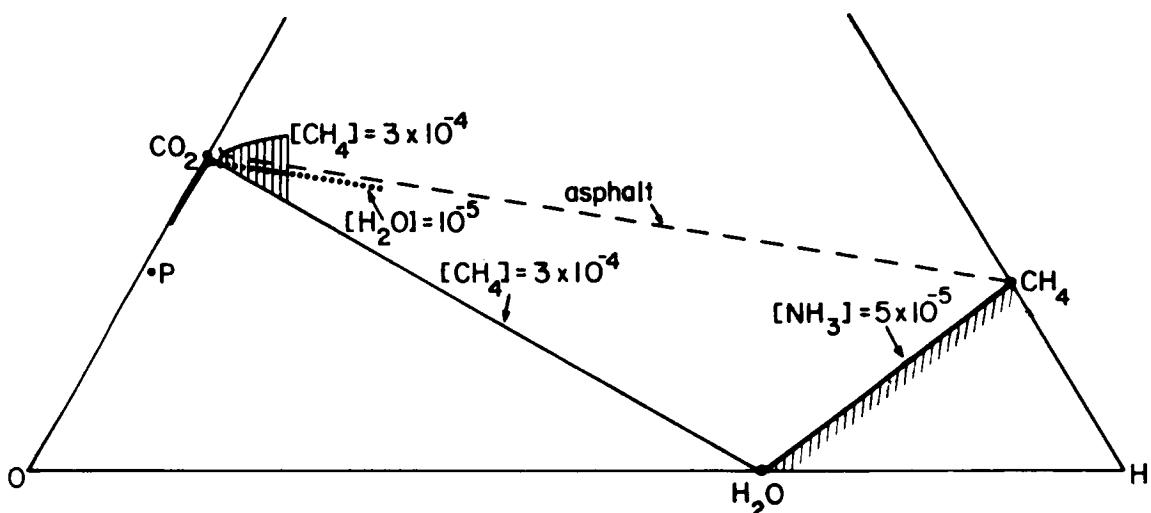


Figure 4. C-H-O ternary diagram for the Martian atmosphere. Areas not excluded by observation are localized about the solid portion of the water line, near the  $\text{CO}_2$  point. One additional abundance determination can specify the thermodynamic equilibrium composition.

mixing ratio imposes a more significant boundary condition, restricting the range of possible atmospheric compositions essentially to the portion below the oxidation threshold, with the exception of a small section of the reducing part of the diagram along the C-O axis. The carbon monoxide upper limit places no new constraint on the diagram; the upper limits on oxygen and ozone eliminate a region near the oxygen corner of the ternary diagram. The estimate for the abundance of water vapor in the Martian atmosphere places the equilibrium composition along a curve which crosses the oxidation threshold not far from the  $\text{CO}_2$  composition point, quite analogous to the situation for Venus. This line quickly enters the region forbidden by the methane abundance upper limits. The composition of the Martian atmosphere is therefore restricted to the solid portion of the water line of Figure 4, encompassing a small region of the oxidizing part of the diagram, and a very small segment, near  $\text{CO}_2$ , in the reducing region.

It has been suggested that various oxides of nitrogen are produced by non-equilibrium processes in the atmosphere of Mars, and that these oxides of nitrogen play a major role in the total chemistry of the atmosphere and surface of Mars (Kiess, Karrer, and Kiess, 1960; 1963). In Table 6, we present some calculations of the equilibrium abundance of various compounds in the Martian atmosphere at representative points in Figure 4. Even in the favorable case where oxygen is present as a major constituent, we see that the resulting abundances of the oxides of nitrogen are extraordinarily small. These conclusions are consistent with those of Sagan, Hanst, and Young (1965), who used a much smaller array of equilibrium reactions than are implicitly included here but who considered also photochemical production and breakdown of these oxides. The present results place the equilibrium upper limit on  $\text{NO}_2$  several orders of magnitude below the previous calculated values (Sagan, Hanst, and Young, 1964); and below the most recent observational upper limits (Marshall, 1964) by the same factor.

Further conclusions on the nature of the Martian atmosphere in thermodynamic equilibrium could be drawn if reliable estimates were performed of the abundances of such molecules as  $\text{CO}$ ,  $\text{CH}_4$ ,  $\text{H}_2\text{S}$ ,  $\text{SO}_3$ ,  $\text{O}_2$ . The limited data available are consistent with the existence of thermodynamic equilibrium, but do not demonstrate thermodynamic equilibrium. As in the case of the atmosphere of Venus, the escape of hydrogen, plus the depletion of atmospheric oxygen (here, either by reaction with the crust or by escape from the planetary exosphere) could have led to an evolutionary track in the ternary diagram approximately along the oxidation threshold. The present information is consistent with a small proportion of molecular oxygen in the atmosphere, although the atmosphere could also be slightly reducing. The possibility of a small quantity of organic molecules on the Martian surface depends in part on which side of the oxidation threshold the total atmospheric composition lies. Note from Table 6 that possibly detectable amounts of  $\text{CH}_4$  and  $\text{H}_2\text{S}$  are allowed in the reducing case.

### Jupiter

The observational constraints on the Jovian atmosphere are shown in Table 7. Because there is no way for water to escape from Jupiter, it must be present in significant amounts below the visible clouds. At the clouds it is frozen out because of the low temperatures. We have arbitrarily assumed that the  $\text{H}_2\text{O}$  mixing ratio below the clouds is comparable to that of methane and ammonia. In the clouds it is fixed by the vapor pressure of ice. The thermodynamic equilibrium calculations were carried out for four sets of pressures and temperatures -- in the first case, for a pressure of 1 atm. and a temperature of  $200^\circ\text{K}$ , corresponding approximately to the region of the clouds (Spinrad and Trafton, 1962; Owen, 1965); and in the second case, for a pressure of 1000 atm. and a temperature of  $350^\circ\text{K}$ . This point corresponds to the level of the hypothesized water droplet clouds, predicted by Gallet (1963; see also Wildt, Smith, Salpeter, and Cameron, 1963). The concentrations of the major resulting constituents of the Jovian atmosphere at the thermodynamic equilibrium are presented in Table 8. The addition of  $10^{-6}$  sulfur would give the other constituents shown. As first pointed out by Wildt (1937), the large

TABLE 5

ADOPTED CHEMICAL COMPOSITION OF THE MARTIAN  
ATMOSPHERE (VOLUME MIXING RATIOS ARE DISPLAYED)

O <sub>3</sub>	<1.3 X 10 <sup>-6</sup>	H <sub>2</sub> S	<2 X 10 <sup>-4</sup>
H <sub>2</sub> O	~10 <sup>-5</sup>	COS	~5 X 10 <sup>-5</sup>
N <sub>2</sub>	~0.9	CO <sub>2</sub>	~1 X 10 <sup>-1</sup>
NO <sub>2</sub>	<3 X 10 <sup>-7</sup>	CH <sub>4</sub>	<3 X 10 <sup>-4</sup>
N <sub>2</sub> O	<5 X 10 <sup>-3</sup>	C <sub>2</sub> H <sub>4</sub>	<5 X 10 <sup>-5</sup>
NH <sub>3</sub>	<5 X 10 <sup>-5</sup>	C <sub>2</sub> H <sub>6</sub>	<3 X 10 <sup>-5</sup>
SO <sub>2</sub>	<1 X 10 <sup>-7</sup>	HCHO	<1 X 10 <sup>-5</sup>
Pressure	~0.05 atm.	Temperature	240°K

(References: Kaplan, Munch, and Spinrad 1964; Owen and Kuiper 1964;  
Hanst and Swan 1965; Chamberlain and Hunten 1965; Marshall 1965)

TABLE 6

THERMODYNAMIC EQUILIBRIUM COMPOSITION OF THE  
MARTIAN ATMOSPHERE, COMPUTED FROM THE  
ELEMENTAL COMPOSITION OF TABLE 5\*

Compound	Oxidizing Case	Slightly Reducing Case
N <sub>2</sub>	0.82	0.90
CO <sub>2</sub>	0.09	0.10
CO	0	3 X 10 <sup>-13</sup>
O <sub>2</sub>	0.09	0
H <sub>2</sub> O	1 X 10 <sup>-5</sup>	1 X 10 <sup>-5</sup>
CH <sub>4</sub>	0	1 X 10 <sup>-6</sup>
C <sub>2</sub> H <sub>6</sub>	0	1 X 10 <sup>-17</sup>
C <sub>6</sub> H <sub>6</sub>	0	0
H <sub>2</sub>	0	1.5 X 10 <sup>-10</sup>
HCHO	0	5 X 10 <sup>-29</sup>
HCOOH	0	4 X 10 <sup>-21</sup>
CH <sub>3</sub> COOH	0	2 X 10 <sup>-18</sup>
CH <sub>3</sub> OH	0	7 X 10 <sup>-27</sup>
NH <sub>3</sub>	0	6 X 10 <sup>-12</sup>
HNO <sub>3</sub>	1 X 10 <sup>-12</sup>	0
NO <sub>2</sub>	6 X 10 <sup>-13</sup>	0
NO	3 X 10 <sup>-20</sup>	0
N <sub>2</sub> O <sub>4</sub>	3 X 10 <sup>-23</sup>	0
N <sub>2</sub> O	1 X 10 <sup>-23</sup>	0
NO <sub>3</sub>	5 X 10 <sup>-27</sup>	0
N <sub>2</sub> O <sub>5</sub>	7 X 10 <sup>-28</sup>	0
N <sub>2</sub> O <sub>3</sub>	2 X 10 <sup>-32</sup>	0
HCN	0	2 X 10 <sup>-29</sup>
SO <sub>3</sub>	1 X 10 <sup>-6</sup>	0
SO <sub>2</sub>	5 X 10 <sup>-22</sup>	5 X 10 <sup>-28</sup>
COS	0	9 X 10 <sup>-10</sup>
H <sub>2</sub> S	0	1 X 10 <sup>-6</sup>
(CH <sub>3</sub> ) <sub>2</sub> SO	0	3 X 10 <sup>-12</sup>
CS <sub>2</sub>	0	1.4 X 10 <sup>-18</sup>
CH <sub>3</sub> SH	0	6 X 10 <sup>-19</sup>
H <sub>2</sub> SO <sub>4</sub>	1 X 10 <sup>-21</sup>	0

\* Two extreme systems, one with [O<sub>2</sub>] = 0, the other with [O<sub>2</sub>] = 0.09 -- corresponding to the point P in Figure 4 -- are displayed. The more highly oxidizing conditions favor the presence of oxides of nitrogen, but even then their predicted equilibrium abundances are minuscule.

TABLE 7  
ADOPTED CHEMICAL COMPOSITION OF THE JOVIAN  
ATMOSPHERE (VOLUME MIXING RATIOS ARE DISPLAYED)

	<u>High</u>	<u>Deep</u>
H <sub>2</sub>	0.60	0.60
H <sub>2</sub> O	$\sim 1 \times 10^{-6}$	$\sim 1 \times 10^{-4}$
NO <sub>2</sub>	$< 3 \times 10^{-6}$	$< 3 \times 10^{-6}$
NH <sub>3</sub>	$2 \times 10^{-4}$	$2 \times 10^{-4}$
CH <sub>4</sub>	$5 \times 10^{-3}$	$5 \times 10^{-3}$
C <sub>2</sub> H <sub>6</sub>	$< 1.2 \times 10^{-4}$	$< 1.2 \times 10^{-4}$
CH <sub>3</sub> NH <sub>2</sub>	$< 3 \times 10^{-4}$	$< 3 \times 10^{-4}$
C <sub>2</sub> H <sub>2</sub>	$< 6 \times 10^{-5}$	$< 6 \times 10^{-5}$
He	0.36	0.36
Ne	0.03	0.03
Pressure	1 atm.	1000 atm.
Temperature	200°K	350°K

(References: Kuiper 1952; Spinrad and Trafton 1963; Owen 1965)

TABLE 8  
THERMODYNAMIC EQUILIBRIUM COMPOSITION OF THE MAJOR  
CONSTITUENTS OF THE JOVIAN ATMOSPHERE, COMPUTED  
FROM THE ELEMENTAL COMPOSITION OF TABLE 7\*

	<u>High</u>	<u>Deep</u>
H <sub>2</sub>	0.60	0.60
He	0.36	0.36
Ne	0.03	0.03
CH <sub>4</sub>	$5 \times 10^{-3}$	$5 \times 10^{-3}$
NH <sub>3</sub>	$2 \times 10^{-4}$	$2 \times 10^{-4}$
H <sub>2</sub> O	$1 \times 10^{-6}$	$1 \times 10^{-4}$
H <sub>2</sub> S	$1 \times 10^{-6}$	$1 \times 10^{-6}$
C <sub>2</sub> H <sub>6</sub>	$3 \times 10^{-23}$	$1 \times 10^{-15}$
N <sub>2</sub>	$6 \times 10^{-22}$	$1 \times 10^{-16}$
CH <sub>3</sub> SH	$2 \times 10^{-28}$	$7 \times 10^{-20}$
CH <sub>3</sub> NH <sub>2</sub>	$2 \times 10^{-31}$	$8 \times 10^{-21}$
CH <sub>3</sub> OH	0	$3 \times 10^{-24}$
(CH <sub>3</sub> ) <sub>2</sub> SO	0	$2 \times 10^{-29}$
CO <sub>2</sub>	0	$1 \times 10^{-31}$
CO	0	$9 \times 10^{-32}$
HCHO	0	$2 \times 10^{-33}$
HCOOH	0	0
HCN	0	0
COS	0	0

\*For the sulfur compounds, addition of [S] =  $10^{-6}$  was assumed.

excess of molecular hydrogen works to greatly reduce the concentration of even simple organic molecules at thermodynamic equilibrium at the lower temperatures. Essentially all carbon is present as methane, all oxygen as water, and all nitrogen as ammonia. The total atmospheric composition gives a point very near the H corner of the ternary diagram. The relative abundance of molecular nitrogen increases fairly rapidly with temperature, but even at 350°K, it is still a very minor atmospheric constituent.

Nevertheless, there is reason to believe that organic molecules may be present in the atmosphere of Jupiter. The bright and contrasting colors of the bands, belts, and spots -- particularly, the Great Red Spot -- surely bethoken differences in molecular composition in the vicinity of the Jovian clouds. The turbulent and shifting appearance of the colors means that they are produced in certain regions, transported, and destroyed in other regions. If the colored compounds were produced by a global thermodynamic equilibrium, they would appear to be perfectly uniform. While some small concentration of minerals may be expected due to micrometeoritic infall, it seems unlikely that such materials are differentially distributed over the Jovian clouds; a more reasonable source of chromophores would appear to arise from the major atmospheric constituents, and therefore, be organic materials (see e.g., Urey, 1952; Sagan, 1963). Experiments attempting to simulate the Jovian atmosphere, in which a mixture of the major gases is supplied with energy from a corona discharge, have succeeded in producing such simple organic molecules as HCN,  $\text{CH}_3\text{CN}$ ,  $\text{C}_2\text{H}_2$ ,  $\text{C}_2\text{H}_4$ , and  $\text{C}_2\text{H}_6$  (Sagan and Miller, 1960). Their interaction products were predicted to be brightly colored. In experiments relevant to the origin of life on Earth, mixtures of materials which are in effect simulated Jovian environments have been subjected to a wide array of energy sources, and organic molecules have been consistently produced in high yield, provided only that the over-all conditions were reducing (see, e.g., Fox, 1965). Electric discharges and solar ultraviolet light -- both leading to high electronic temperatures of the excited atoms and both to be expected in the vicinity of the Jovian clouds -- will lead to the production of organic molecules by thermodynamic equilibrium processes.

In a further theoretical test of this contention, we have found that, over a wide range of pressures and temperatures, it is possible to find conditions where polycyclic aromatic compounds are formed in significant quantities for a rapidly quenched system of Jovian composition. In Table 9 are displayed two typical systems: the first, at 1 atm. and 1500°K, is intended to represent electrical discharges in the upper (visible) Jovian clouds; the second, at  $10^{-6}$  atm. and 1000°K, a hypothetical Jovian thermosphere from which complex organic material rapidly diffuses to lower altitudes. The five most abundant predicted compounds synthesized in the former case are exactly the compounds experimentally produced by corona discharge in the Jovian simulation experiment of Sagan and Miller (1960). In these sample calculations highly colored compounds (such as azulene, asphalt, and azobenzene) are synthesized, as had also been predicted. Thus equilibrium thermodynamics alone tends to produce complex organic compounds -- some of them highly colored -- provided that an intermittent source of high temperature exists.

TABLE 9  
PREDICTED EQUILIBRIUM IN THE JOVIAN ATMOSPHERE  
AT HIGH TEMPERATURES AND MODERATE TO  
LOW PRESSURES

Pressure	$\sim 1$ atm.	$\sim 10^{-6}$ atm.
Temperature	1500°K	1000°K
Noble gases	0.4	0.4
H <sub>2</sub>	0.6	0.6
CH <sub>4</sub>	$4 \times 10^{-3}$	$6 \times 10^{-5}$
C <sub>2</sub> H <sub>2</sub>	$2 \times 10^{-4}$	$2 \times 10^{-3}$
C <sub>2</sub> H <sub>4</sub>	$3 \times 10^{-5}$	$7 \times 10^{-7}$
C <sub>2</sub> H <sub>6</sub>	$2 \times 10^{-7}$	$1 \times 10^{-2}$
Benzene	$2 \times 10^{-9}$	$1 \times 10^{-7}$
Naphthalene	$1 \times 10^{-12}$	$4 \times 10^{-9}$
Asphalt (yellow)	$6 \times 10^{-25}$	$1 \times 10^{-8}$
N <sub>2</sub>	$7 \times 10^{-5}$	$6 \times 10^{-5}$
HCN	$6 \times 10^{-5}$	$9 \times 10^{-5}$
NH <sub>3</sub>	$2 \times 10^{-7}$	$2 \times 10^{-13}$
CH <sub>3</sub> CN	$6 \times 10^{-8}$	$2 \times 10^{-10}$
Azulene (blue)	$5 \times 10^{-14}$	$2 \times 10^{-9}$
Aniline	$3 \times 10^{-19}$	$2 \times 10^{-23}$
Azobenzene (red)	$3 \times 10^{-28}$	$3 \times 10^{-33}$

The formation of graphite was excluded. High temperatures produced by lightning could permit approach to such equilibria, followed by rapid quenching. Polynuclear aromatics and colored compounds such as azulene tend to form.

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**Appendix II**

**Thermodynamic Equilibrium**

**and the Inorganic Origin of**

**Organic Compounds**

## APPENDIX II

### THERMODYNAMIC EQUILIBRIUM AND THE INORGANIC ORIGIN OF ORGANIC COMPOUNDS

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#### Abstract

Theoretical and experimental support is presented for the hypothesis that many organic compounds may form under conditions of thermodynamic equilibrium. This possibility must be considered along with special effects of selective catalysts, radiation, and degradation from biological matter, in explaining the origin of organic compounds in carbonaceous chondrites. Similar considerations may apply to solar nebulae and planetary atmospheres. The equilibrium distribution of organic compounds at temperatures between 300°K and 1000°K and pressures of  $10^{-6}$  to 50 atm. for the C-H-O system have been computed. At moderate temperatures and low pressures, conditions where graphite production is inhibited, aromatic compounds may form even in the presence of large excesses of hydrogen. Such conditions exist in the solar nebula and in the atmospheres of some of the major planets. Equilibrium concentrations of a large number of compounds at 1000°K with N, S, and Cl added to the system have also been determined. In some cases, a limited equilibrium method is employed in which those few compounds which form with the most difficulty are excluded from the computations, while representatives of all other families of compounds are included. This approach is shown to be useful in the interpretation of certain experimental data in which complete equilibrium has not been attained. We have also found that gases, activated to the plasma state by a high energy radio frequency field, recombine on cooling to yield product mixtures which are in qualitative agreement with those predicted by the equilibrium computations. We believe that such products can be profitably studied as if at a metastable limited equilibrium.

#### Introduction

In studies of the origin of organic mixtures such as asphalt, petroleum or the organic substances found in carbonaceous meteorites<sup>(1-6)</sup>, it is important to account for the relative amounts of the various compounds present. Studier, Hayatsu and Anders<sup>(1)</sup>, who have analyzed a number of carbonaceous chondrites by mass spectrometry, have proposed that the organic compounds they identified may have been formed under equilibrium or near equilibrium conditions in a solar nebula. They hold that neither biological process nor high

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energy radiation (without the influence of thermodynamic equilibration) could account for their observed proportions of compounds, particularly the preponderance of aromatic hydrocarbons and the high methane-to-ethane ratio. Their data did agree rather well, however, with a typical distribution calculated by Dayhoff, Lippincott and Eck<sup>(7)</sup> for conditions of thermodynamic equilibrium for a C-H-O-N ideal gas system. Urey and Lewis<sup>(8)</sup> on the other hand object to the hypothesis of an equilibrium origin of such compounds in the absence of graphite and maintain that the organic compounds detected by Studier et al., and other investigators in meteorites, could only have been produced by high-energy radiation or, in some instances, by living organisms. In subsequent communications Studier, Hayatsu and Anders<sup>(9)</sup> reported support for the equilibrium theory by the identification of products formed experimentally from carbon monoxide and hydrogen using heat alone, or with meteoritic material or inorganic compounds as catalysts.

The interest in this topic has led us to extend the scope of our computations in three ways: to include a larger number of elements and compounds, to widen the range of temperatures and pressures considered, and to take into account metastable conditions or limited thermodynamic equilibrium in which there is insufficient time for full equilibrium to be attained. These more general computations have led to some interesting new concepts concerning the application of equilibrium to planetary atmospheres and solar nebulae.

In our previous paper<sup>(7)</sup> we presented the calculated distribution of elements among over 100 compounds at 1 atm. pressure and 500°K. At some C-H-O elemental proportions the formation of graphite was excluded because of the high activation energy of all reactions forming it. The present report describes calculations of thermodynamic equilibria in C-H-O systems at temperatures from 300°K to 1000°K and pressures from  $10^{-6}$  to 50 atmospheres. Additional calculations including the elements N, S, and Cl at 1000°K are reported. Preliminary experiments on equilibria produced in a plasma discharge system are also presented.

The distribution of molecular species at chemical equilibrium is independent of the specific reactions by which that equilibrium is reached. There need be only one reversible reaction pathway from the major constituents that will produce each compound. At thermodynamic equilibrium, the equilibrium constants for all possible reactions among the constituents are simultaneously satisfied. The compound concentrations in an ideal gas mixture at equilibrium then depend only on the pressure, temperature and elemental composition of the system, on the compounds assumed to be present in the system, and on the standard free energy of formation and molecular formula of each such compound.

The difficulties previously limiting the simultaneous computation of concentrations of many organic compounds were overcome by using a high speed computer. The general method of White, Johnson and Dantzig<sup>(10)</sup> was followed. By an iterative process, that distribution of species is found which minimizes the total free energy of the system while simultaneously satisfying the constraints on total elemental composition. At each stage  $M + 1$  linear equations are solved where  $M$  is the number of elements in the system.

The standard free energies of formation for the compounds were obtained from tables based on experimental results or by the method of group contributions suggested by van Krevelen and Chermin<sup>(11)</sup>. In this latter method, advantage is taken of the fact that the free energy of an organic compound is nearly a sum of "group contributions" from its constituent bonds, branch points, its rings and symmetry numbers. Free energy values for each group are derived from experimental values for a few compounds which contain it. The precision of the calculated free energies is within 2 kcal/mole for compounds similar to those measured and is usually much closer. The values for the major constituents  $\text{CO}_2$ ,  $\text{CH}_4$ ,  $\text{H}_2\text{O}$  and  $\text{CO}$  are known much more precisely. If the free energy used for a minor compound is too high by 1 kcal, the concentration calculated will be too small by a factor of .36 at 500°K and .60 at 1000°K.

A detailed description of the method, tabulation and documentation of free energy values and presentation and discussion of results is given in Chapter 2.

### C H O Systems

In the general ternary diagram (Fig. 1) the main characteristics of ideal gas systems containing all proportions of the elements C, H, and O are shown. There are two pronounced thresholds at which concentrations of many compounds change abruptly by many orders of magnitude. The first is the oxidizing threshold along the  $\text{CO}_2$ - $\text{H}_2\text{O}$  line, below which free  $\text{O}_2$  appears and all organic compounds are oxidized; above this line traces of many organics appear in addition to  $\text{CO}_2$ ,  $\text{CO}$ ,  $\text{H}_2\text{O}$  and  $\text{CH}_4$ . The second is the "asphalt" threshold above which large concentrations of benzene and polynuclear aromatics appear. The position of this line varies with temperature and pressure, in contrast to the oxidizing threshold which remains essentially unchanged. There is a weak hydrogen threshold along the  $\text{CH}_4$ - $\text{H}_2\text{O}$  line which appears at low temperatures. For example, at 500°K and 1 atm.,  $\text{CO}$ ,  $\text{CO}_2$ , benzene, ethane, hexane,  $\text{CS}_2$ ,  $\text{COS}$ , etc. vary by several orders of magnitude in crossing this line. The curved line represents a phase boundary above which solid graphite would precipitate in a complete equilibrium.

The positions of the graphite phase boundary at various temperatures and pressures are shown in Figure 2. In addition to the data illustrated, it may be noted that at 500°K and  $10^{-6}$  atm. and at 700°K at both  $10^{-6}$  and  $10^{-3}$  atm. this line ends near the hydrogen corner.

Conventional equilibrium computations consider a very limited number of compounds, usually in single, reversible reactions. The balance of chemical species is computed for this extremely limited system as if no other reactions were occurring at the same time. Organic chemists know that this is frequently highly unrealistic; such a simplification is justified by necessity because more complex systems could not be considered in detail. With the use of high-speed digital computers, routine calculations of simultaneous reactions among a very large number of compounds is possible. In practical cases where time is important, complete equilibrium may be an unrealistic

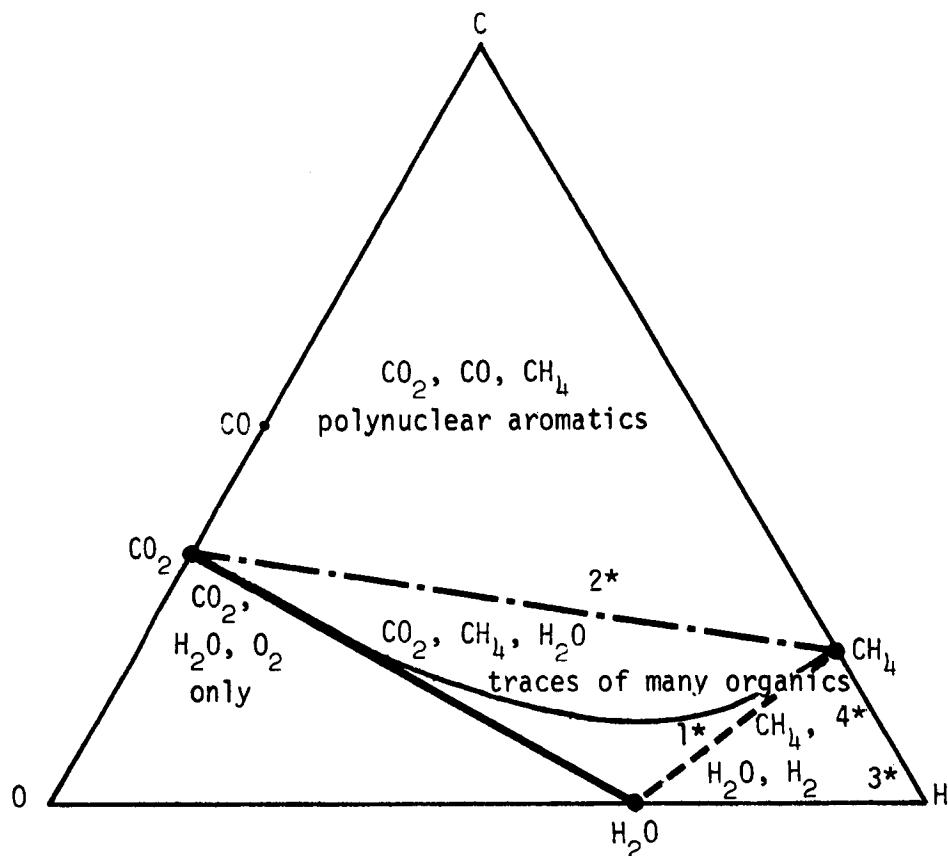


Fig. 1. Thermodynamic equilibria in atmospheres of varying elemental proportions. The ternary diagram provides a display of systems of all possible relative proportions of C, H, and O. The points corresponding to pure gases of the major compounds are indicated, and regions where different compounds are important are shown. The solid curve indicates the phase boundary along which graphite becomes stable at 1 atm. and 500°K. The activation energy for this reaction is so high that under many conditions it does not occur and gaseous equilibria above this line are observed experimentally. Above the line CH<sub>4</sub>-CO<sub>2</sub>, equilibrium favors the formation of large proportions of polycyclic aromatic compounds and a lesser increase in most of the other families of compounds. The graphite and asphalt lines are always present, but their positions vary with temperature and pressure. The numbered asterisks indicate the compositions of the equilibrium distributions shown in Table 1.

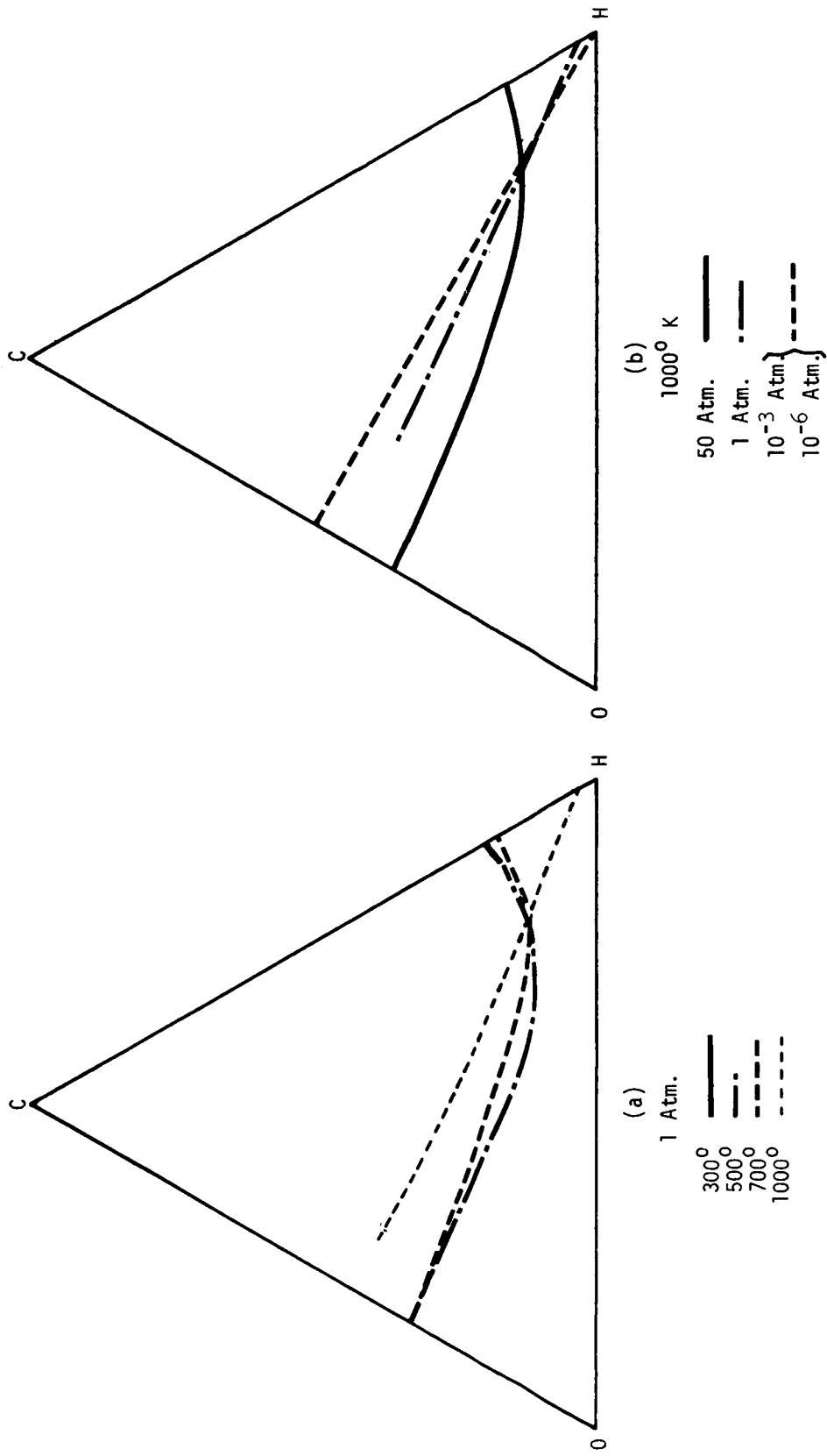


Figure 2. Graphite phase boundaries. In an all-inclusive equilibrium, the gas phase would never have a position above this phase boundary. However, the activation energy barrier to graphite formation is very high so that under many conditions equilibrium may be approximated in metastable gases without any graphite formation. At 300°K a liquid water phase forms over the lower central portion of the figure. Outside this region, the graphite phase boundary is indistinguishable from the boundary at 500°K.

ideal. With rapid quenching, or at temperatures at which reactions require appreciable lengths of time to approach equilibrium, some reactions may occur only to a negligible extent. If the activation energy for all reactions leading to a particular product is high, and the temperature is sufficiently low, this product may be essentially "forbidden". All the other compounds of the system may have reached a metastable equilibrium after a certain time, while the particular compound is still present only in very small amounts.

#### Method of Limited Equilibrium, Exclusion of Graphite

As a way of simulating such conditions for purposes of computation, we use a method of limited equilibrium, in which all compounds of significant concentration are included except the few which are specifically excluded. In these calculations, the rate of production of each compound is assumed to be either rapid enough for equilibrium to be approximated, or negligible (zero). Experiments show that some reactions are indeed inhibited on a time scale of days at temperatures as high as 850°K<sup>(9)</sup>. It should be noted that the actual production of small amounts of the forbidden compounds does not seriously disturb the proportions of the compounds in the quasi-equilibrium mixture. The method is a valid approximation as long as the forbidden compounds do not approach their final equilibrium concentrations.

According to a formally strict definition of thermodynamic equilibrium, graphite must be included as a major constituent of the system<sup>(8,12,13)</sup>. However at some temperatures, there are reasons to exclude graphite from the computation and to use the method of limited equilibrium. Graphite is the end product of the polymerization of higher aromatic compounds, a relatively long sequence of reactions. At temperatures below about 850°K, it apparently cannot form directly from methane and other simple organics on a laboratory time scale, because the activation energy of such reactions would be too high. At lower temperatures as in petroleum deposits, the metastability persists on a geological time scale. At moderate temperatures, therefore, a metastable equilibrium of many other compounds could be approached before significant amounts of graphite could be produced. The elemental proportions represented by the region above the graphite line in the ternary diagram therefore give gas-phase compositions which can actually be attained experimentally. The exclusion of graphite permits these compositions to be studied, and the "asphalt region" to be investigated. If we had felt obliged to adhere to the strict definition of "equilibrium", many of these studies could not have been carried out. In some of the following computations, graphite has been excluded.

In Figure 3 are shown boundaries above which the benzene concentration is greater than  $10^{-6}$  mole fraction, an amount readily measured experimentally. At high temperatures and low pressures, benzene (and asphalt) appear even in an atmosphere containing a large excess of free hydrogen. This point is significant in theories concerning the formation of organic compounds in gas mixtures containing large excesses of hydrogen. Our result is consistent with the experimental findings of Studier et al<sup>(9)</sup> who have proposed that such conditions may have existed in solar nebulae<sup>(1)</sup>. The formation of asphalt in the presence of excess hydrogen is due to two mutually reinforcing factors.

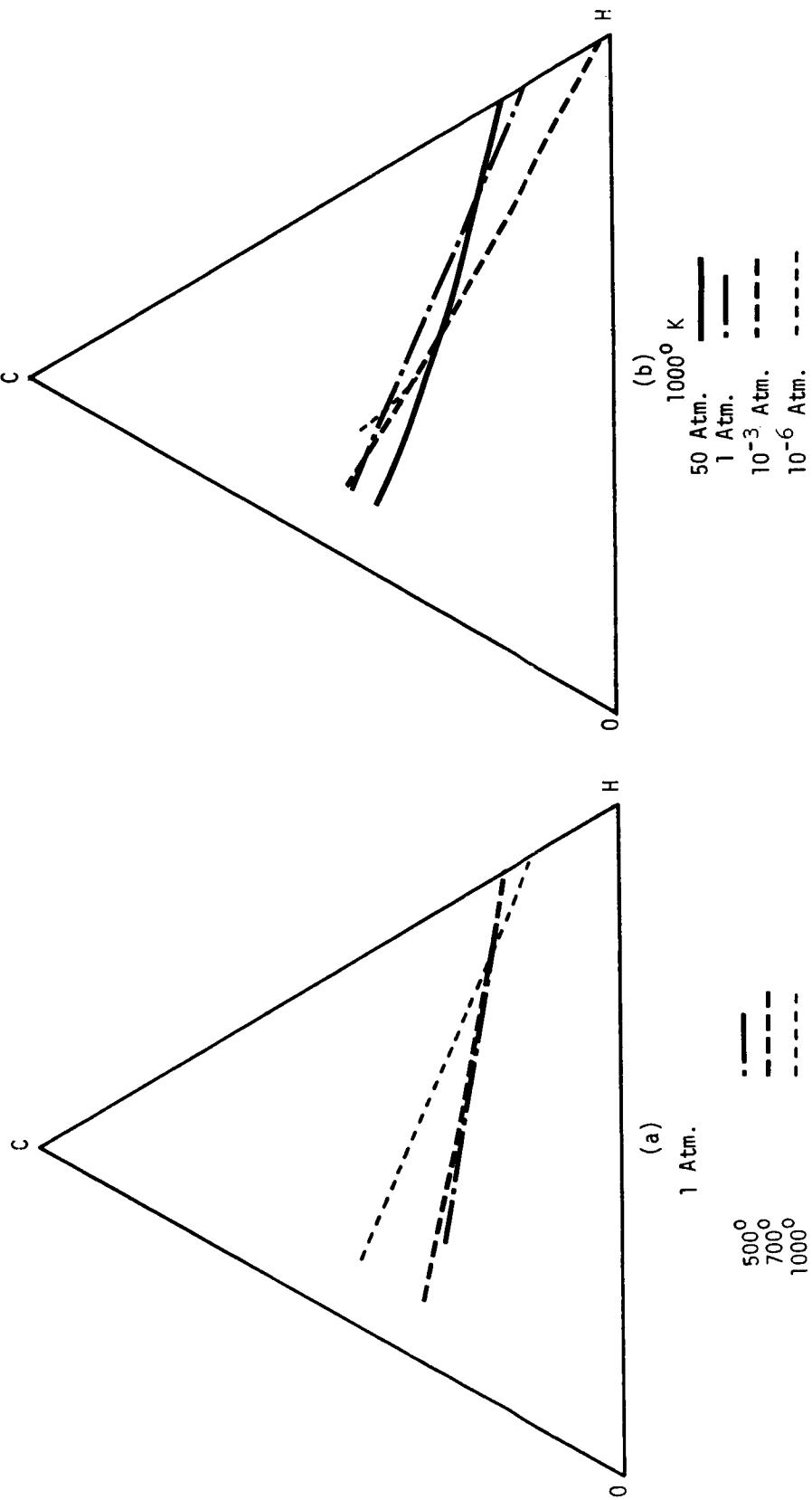
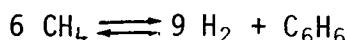


Figure 3. Curves where benzene concentration is  $10^{-6}$  mole fraction. Benzene is found at  $1000^{\circ}\text{K}$  even in the presence of an excess of hydrogen. The curves for 50 atm and 1 atm at  $1000^{\circ}\text{K}$  are indistinguishable except for a slight divergence at the upper end. At  $300^{\circ}\text{K}$  the benzene concentration is slightly lower than  $10^{-6}$  atm above the  $\text{CO}_2\text{-CH}_4$  line and much lower elsewhere.

Firstly methane, a major constituent, becomes less stable with increasing temperature. Secondly, the equation



shifts toward the right as the pressure decreases. Benzene and asphalt become measurable only in regions where solid graphite would be stable if it had been included in the equilibrium.

With graphite formation excluded, the concentrations of the other constituents change only gradually in the neighborhood of the graphite line; it is not a definite "threshold". Above the graphite line there are regions where the computed benzene concentration would become very high if benzene were the only aromatic included in the equilibrium. When higher molecular weight aromatics are included also, they become more important than benzene. The largest polynuclear aromatics often become so concentrated that they would precipitate. However, since the large molecules must build up from the small ones, the kinetics of a given situation dictate how far this polymerization will be able to go in the available time. We have approximated the condensation of polynuclear aromatics by including in our computation benzene, naphthalene, and a mixture we call "asphalt", which is a composite of 100 isomers having six benzene rings with the molecular formula  $\text{C}_{22}\text{H}_{12}$ . The free energy of this composite is computed by the method of group contributions<sup>(11)</sup>. For each temperature and pressure the position of the asphalt threshold, where aromatics build up sharply, is insensitive to the exact formulas and free energies of the aromatics included in the equilibria. The threshold is sharper at lower temperatures and at higher pressures. Figure 4 shows lines above which the asphalt concentration is greater than  $10^{-6}$  mole fraction for various conditions of temperature and pressure. Asphalt may form at all temperatures and pressures investigated. At high temperature and low pressure it is stable even in the hydrogen-rich region.

#### C,H,O,N,S,P,Cl Systems

In the study of meteorites and geological deposits, the elements N, S, and Cl are also important. The addition of an amount of N equal to that of C produces very little change in the system. Molecular nitrogen remains principally as  $\text{N}_2$  forming only traces of organics and oxides, a small amount of  $\text{NH}_3$  in the presence of excess  $\text{H}_2$ , and a little HCN in the asphalt region. Formation of HCN is particularly favored by low pressure.  $\text{NH}_3$  is favored by low temperature, high pressure, and high hydrogen concentration. In the atmosphere of Jupiter, it is the main nitrogen-containing compound. Rapid change of such a system might lead to products of a limited equilibrium in which  $\text{N}_2$  did not participate. This would produce a relative increase in the concentrations of all other nitrogenous compounds.

Table I shows the mole fraction abundances of various compounds of interest at a temperature of  $1000^\circ\text{K}$  and pressures of 1 and  $10^{-6}$  atm. The molar

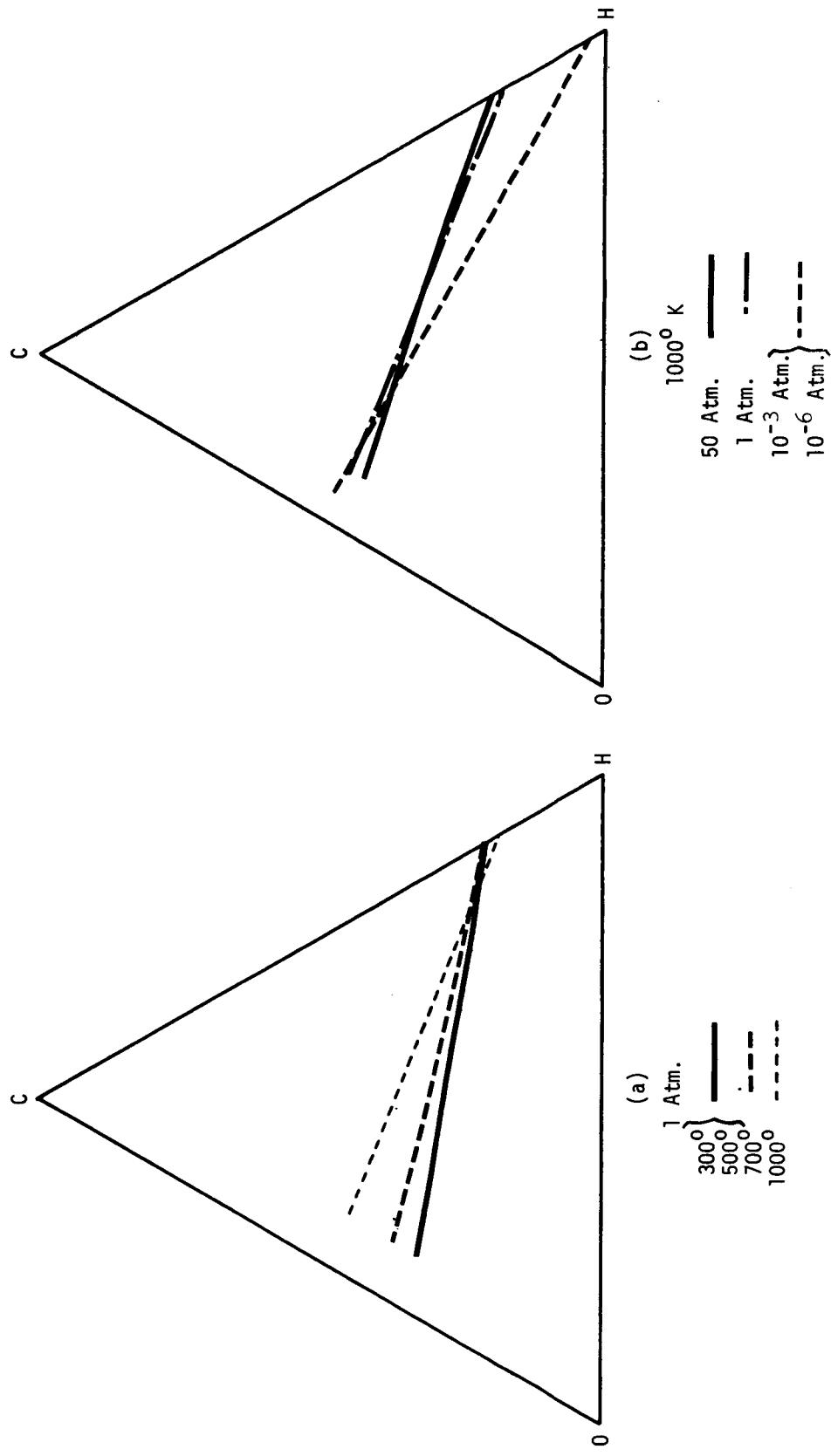


Figure 4. Curves above which asphalt concentration is greater than  $10^{-6}$  mole fraction. Graphite has been omitted from these systems for kinetic reasons. At 300°K the curves for pressures from  $10^{-6}$  to 50 atm are very close together. Asphalt forms at all temperatures and pressures investigated. At high temperature and low pressure it is stable even where excess H<sub>2</sub> is present.

TABLE I. MOLE FRACTION COMPOSITIONS OF COMPOUNDS IN EQUILIBRIUM

The relative abundances of C, H and O for the four points are shown in Fig. 1. N is as abundant as carbon. Cl and S are 1.0 % as abundant as C. Temperatures of 1000°K and pressures of 1 atm. or  $10^{-6}$  atm. are considered.

Elemental Composition Point (See Fig. 1)	1 Atm.				$10^{-6}$ Atm.			
	1	2	3	4	1	2	3	4
H <sub>2</sub>	.54	.11	.86	.55	.55	.37	.91	.81
O <sub>2</sub>	.59x10 <sup>-21</sup>	.57x10 <sup>-26</sup>	.15x10 <sup>-23</sup>	.37x10 <sup>-25</sup>	.52x10 <sup>-15</sup>	.99x10 <sup>-35</sup>	.25x10 <sup>-36</sup>	.21x10 <sup>-36</sup>
H <sub>2</sub> O	.15	.92x10 <sup>-4</sup>	.12x10 <sup>-1</sup>	.12x10 <sup>-2</sup>	.15	.14x10 <sup>-10</sup>	.53x10 <sup>-11</sup>	.43x10 <sup>-11</sup>
CO <sub>2</sub>	.55x10 <sup>-1</sup>	.48x10 <sup>-3</sup>	.56x10 <sup>-3</sup>	.15x10 <sup>-3</sup>	.53x10 <sup>-1</sup>	.17x10 <sup>-10</sup>	.32x10 <sup>-12</sup>	.30x10 <sup>-12</sup>
CO	.14	.40	.28x10 <sup>-1</sup>	.48x10 <sup>-1</sup>	.15	.34	.39x10 <sup>-1</sup>	.41x10 <sup>-1</sup>
CH <sub>4</sub>	.55x10 <sup>-2</sup>	.19	.55x10 <sup>-1</sup>	.25	.63x10 <sup>-14</sup>	.49x10 <sup>-4</sup>	.21x10 <sup>-3</sup>	.19x10 <sup>-3</sup>
C <sub>2</sub> H <sub>6</sub>	.11x10 <sup>-7</sup>	.68x10 <sup>-4</sup>	.70x10 <sup>-6</sup>	.22x10 <sup>-4</sup>	.14x10 <sup>-31</sup>	.13x10 <sup>-11</sup>	.96x10 <sup>-11</sup>	.89x10 <sup>-11</sup>
N <sub>2</sub>	.10	.30	.42x10 <sup>-1</sup>	.15	.10	.25	.37x10 <sup>-1</sup>	.12
NH <sub>3</sub>	.69x10 <sup>-4</sup>	.10x10 <sup>-4</sup>	.89x10 <sup>-4</sup>	.86x10 <sup>-4</sup>	.70x10 <sup>-10</sup>	.62x10 <sup>-10</sup>	.91x10 <sup>-10</sup>	.14x10 <sup>-9</sup>
HCN	.41x10 <sup>-6</sup>	.28x10 <sup>-3</sup>	.13x10 <sup>-5</sup>	.21x10 <sup>-4</sup>	.45x10 <sup>-12</sup>	.10x10 <sup>-1</sup>	.43x10 <sup>-2</sup>	.82x10 <sup>-2</sup>
Benzene	.20x10 <sup>-18</sup>	.76x10 <sup>-3</sup>	.29x10 <sup>-14</sup>	.12x10 <sup>-8</sup>	<10 <sup>-38</sup>	.28x10 <sup>-5</sup>	.53x10 <sup>-5</sup>	.84x10 <sup>-5</sup>
Naphthalene	.88x10 <sup>-30</sup>	.41x10 <sup>-3</sup>	.48x10 <sup>-23</sup>	.18x10 <sup>-13</sup>	<10 <sup>-38</sup>	.11x10 <sup>-5</sup>	.13x10 <sup>-5</sup>	.31x10 <sup>-5</sup>
"Asphalt"	<10 <sup>-38</sup>	.33x10 <sup>-4</sup>	<10 <sup>-38</sup>	.46x10 <sup>-29</sup>	<10 <sup>-38</sup>	.68x10 <sup>-2</sup>	.86x10 <sup>-3</sup>	.80x10 <sup>-2</sup>
Formic acid	.15x10 <sup>-7</sup>	.26x10 <sup>-10</sup>	.25x10 <sup>-9</sup>	.42x10 <sup>-10</sup>	.15x10 <sup>-13</sup>	.33x10 <sup>-23</sup>	.15x10 <sup>-24</sup>	.13x10 <sup>-24</sup>
Acetic acid	.24x10 <sup>-10</sup>	.70x10 <sup>-11</sup>	.24x10 <sup>-11</sup>	.28x10 <sup>-11</sup>	.26x10 <sup>-28</sup>	.66x10 <sup>-28</sup>	.52x10 <sup>-29</sup>	.44x10 <sup>-29</sup>
Formaldehyde	.10x10 <sup>-6</sup>	.54x10 <sup>-7</sup>	.32x10 <sup>-7</sup>	.34x10 <sup>-7</sup>	.10x10 <sup>-12</sup>	.17x10 <sup>-12</sup>	.47x10 <sup>-13</sup>	.43x10 <sup>-13</sup>
Methanol	.24x10 <sup>-8</sup>	.25x10 <sup>-9</sup>	.12x10 <sup>-8</sup>	.85x10 <sup>-9</sup>	.26x10 <sup>-20</sup>	.28x10 <sup>-20</sup>	.19x10 <sup>-20</sup>	.16x10 <sup>-20</sup>
Ethanol	.34x10 <sup>-13</sup>	.63x10 <sup>-12</sup>	.11x10 <sup>-12</sup>	.52x10 <sup>-13</sup>	.41x10 <sup>-37</sup>	.50x10 <sup>-27</sup>	.60x10 <sup>-27</sup>	.50x10 <sup>-27</sup>
Ethylene	.72x10 <sup>-8</sup>	.22x10 <sup>-3</sup>	.28x10 <sup>-6</sup>	.14x10 <sup>-4</sup>	.90x10 <sup>-26</sup>	.12x10 <sup>-5</sup>	.36x10 <sup>-5</sup>	.38x10 <sup>-5</sup>
Acetylene	.27x10 <sup>-10</sup>	.42x10 <sup>-5</sup>	.65x10 <sup>-9</sup>	.49x10 <sup>-7</sup>	.33x10 <sup>-22</sup>	.64x10 <sup>-2</sup>	.80x10 <sup>-2</sup>	.93x10 <sup>-2</sup>
Xylene	.16x10 <sup>-27</sup>	.19x10 <sup>-7</sup>	.88x10 <sup>-22</sup>	.18x10 <sup>-14</sup>	<10 <sup>-38</sup>	.37x10 <sup>-18</sup>	.21x10 <sup>-17</sup>	.35x10 <sup>-17</sup>
Acetone	.97x10 <sup>-15</sup>	.16x10 <sup>-10</sup>	.12x10 <sup>-13</sup>	.63x10 <sup>-12</sup>	<10 <sup>-38</sup>	.27x10 <sup>-24</sup>	.23x10 <sup>-24</sup>	.22x10 <sup>-24</sup>
Dimethyl ether	.81x10 <sup>-13</sup>	.15x10 <sup>-11</sup>	.26x10 <sup>-12</sup>	.12x10 <sup>-11</sup>	.97x10 <sup>-37</sup>	.12x10 <sup>-26</sup>	.14x10 <sup>-26</sup>	.12x10 <sup>-26</sup>
Methylamine	.23x10 <sup>-11</sup>	.58x10 <sup>-10</sup>	.18x10 <sup>-10</sup>	.12x10 <sup>-9</sup>	.26x10 <sup>-29</sup>	.26x10 <sup>-19</sup>	.67x10 <sup>-19</sup>	.10x10 <sup>-18</sup>
Glycine	.88x10 <sup>-20</sup>	.20x10 <sup>-20</sup>	.73x10 <sup>-21</sup>	.13x10 <sup>-20</sup>	<10 <sup>-38</sup>	<10 <sup>-38</sup>	<10 <sup>-38</sup>	<10 <sup>-38</sup>
Pyridine	.81x10 <sup>-22</sup>	.14x10 <sup>-8</sup>	.15x10 <sup>-18</sup>	.14x10 <sup>-13</sup>	<10 <sup>-38</sup>	.12x10 <sup>-12</sup>	.77x10 <sup>-13</sup>	.20x10 <sup>-12</sup>
S <sub>2</sub>	.74x10 <sup>-9</sup>	.12x10 <sup>-6</sup>	.50x10 <sup>-10</sup>	.15x10 <sup>-8</sup>	.32x10 <sup>-3</sup>	.88x10 <sup>-7</sup>	.18x10 <sup>-7</sup>	.51x10 <sup>-7</sup>
CS <sub>2</sub>	.12x10 <sup>-8</sup>	.17x10 <sup>-3</sup>	.31x10 <sup>-9</sup>	.98x10 <sup>-7</sup>	.55x10 <sup>-9</sup>	.26x10 <sup>-2</sup>	.39x10 <sup>-3</sup>	.12x10 <sup>-2</sup>
H <sub>2</sub> S	.20x10 <sup>-2</sup>	.50x10 <sup>-2</sup>	.84x10 <sup>-3</sup>	.29x10 <sup>-2</sup>	.14x10 <sup>-2</sup>	.15x10 <sup>-4</sup>	.17x10 <sup>-4</sup>	.25x10 <sup>-4</sup>
SO <sub>2</sub>	.20x10 <sup>-10</sup>	.25x10 <sup>-14</sup>	.14x10 <sup>-13</sup>	.18x10 <sup>-14</sup>	.12x10 <sup>-4</sup>	.37x10 <sup>-26</sup>	.44x10 <sup>-28</sup>	.59x10 <sup>-28</sup>
COS	.17x10 <sup>-4</sup>	.59x10 <sup>-3</sup>	.87x10 <sup>-6</sup>	.80x10 <sup>-5</sup>	.11x10 <sup>-4</sup>	.44x10 <sup>-6</sup>	.23x10 <sup>-7</sup>	.40x10 <sup>-7</sup>
Methanethiol	.20x10 <sup>-8</sup>	.86x10 <sup>-6</sup>	.51x10 <sup>-8</sup>	.13x10 <sup>-6</sup>	.15x10 <sup>-20</sup>	.19x10 <sup>-12</sup>	.38x10 <sup>-12</sup>	.57x10 <sup>-12</sup>
Benzenethiol	.12x10 <sup>-23</sup>	.56x10 <sup>-7</sup>	.45x10 <sup>-20</sup>	.10x10 <sup>-13</sup>	<10 <sup>-38</sup>	.18x10 <sup>-12</sup>	.16x10 <sup>-12</sup>	.41x10 <sup>-12</sup>
Thiophene	.20x10 <sup>-17</sup>	.63x10 <sup>-6</sup>	.32x10 <sup>-15</sup>	.98x10 <sup>-11</sup>	<10 <sup>-38</sup>	.13x10 <sup>-8</sup>	.92x10 <sup>-9</sup>	.21x10 <sup>-8</sup>
Cl <sub>2</sub>	.24x10 <sup>-15</sup>	.11x10 <sup>-13</sup>	.26x10 <sup>-16</sup>	.50x10 <sup>-15</sup>	.23x10 <sup>-15</sup>	.23x10 <sup>-14</sup>	.22x10 <sup>-16</sup>	.24x10 <sup>-15</sup>
HCl	.20x10 <sup>-2</sup>	.59x10 <sup>-2</sup>	.84x10 <sup>-3</sup>	.29x10 <sup>-2</sup>	.20x10 <sup>-2</sup>	.51x10 <sup>-2</sup>	.77x10 <sup>-3</sup>	.24x10 <sup>-2</sup>
CH <sub>3</sub> Cl	.69x10 <sup>-9</sup>	.36x10 <sup>-6</sup>	.18x10 <sup>-8</sup>	.44x10 <sup>-7</sup>	.77x10 <sup>-21</sup>	.23x10 <sup>-10</sup>	.61x10 <sup>-11</sup>	.19x10 <sup>-10</sup>
CCl <sub>4</sub>	.35x10 <sup>-33</sup>	.62x10 <sup>-27</sup>	.16x10 <sup>-34</sup>	.63x10 <sup>-31</sup>	<10 <sup>-38</sup>	.58x10 <sup>-33</sup>	.38x10 <sup>-37</sup>	.51x10 <sup>-35</sup>

abundances of the new elements relative to carbon were  $[N] = [C]$ ,  $[S] = .0001 X [C]$ , and  $[Cl] = .0001 X [C]$ . Mole fractions of constituents at the elemental composition points 1, 2, 3 and 4, shown in Fig. 1, are tabulated in Table I. Point 1 is chosen below the graphite phase boundary and represents a strict, all-inclusive equilibrium. At the other three points, solid graphite formation was forbidden at 1000°K. It may be seen from the table that asphalt formation is encouraged by low pressure, so that it forms readily even in a system with a large excess of  $H_2$ . Low pressure also favors the decomposition of  $CH_4$ ,  $CO_2$ , and  $NH_3$ .

In the asphalt region HCN and acetylene concentrations build up, as well as those of aromatics. Pyridine, the most stable of the nitrogen-containing aromatics is always less concentrated than benzene by several orders of magnitude.

The principal compound containing chlorine is  $HC1$ . Chloromethane, the most stable chlorinated hydrocarbon, is considerably less stable.

The most important sulphur compound is  $H_2S$  except at low pressure in the asphalt region where  $CS_2$  is most important. Generally, organic sulphur compounds are much more stable than their oxygen analogs. This peculiarity may become important in theories of the origin of life. Carbon disulphide, methanethiol, benzenethiol, and thiophene are among the most stable sulphur-containing compounds.

#### Application to Observed Data

The ethane-methane ratio is of interest since this ratio was found to be  $10^{-3}$  or less in some carbonaceous chondrites. It is smaller than that observed in fossil fuels or in photoactivated polymerizations or cracking processes<sup>(1)</sup>. This ratio was computed to be less than  $10^{-3}$  for all points illustrated in Table I.

In the Fischer-Tropsch synthesis of hydrocarbons, the temperature can be kept low enough so that benzene does not form readily, presumably because the activation energies of all reactions leading to it are too high. In accordance with the method of limited equilibrium, we have therefore made computations in an otherwise all-inclusive system from which graphite, benzene, and all aromatic compounds are deleted. This leads to significant proportions of aliphatic compounds. A comparison of systems with and without aromatics is shown in Table II. When aromatics are omitted, cyclopentane and cyclohexane are important. The larger aliphatic hydrocarbons are much more concentrated in this case than when benzene is present -- the higher homolog mole fractions decreasing by a factor of ten for each additional carbon in the chain. Hydrocarbons with one double bond are slightly less stable than saturated ones. Those with a triple bond are considerably less stable. The ethane-to-methane ratio is .014. In the computed equilibrium, there is little difference in concentration between normal isomers and branched chains, in contrast to the preference for normal isomers experimentally observed in the Fischer-Tropsch

TABLE II. MOLE FRACTION COMPOSITION OF GAS MIXTURE C:H:O=30:40:30 AT 1 ATM. PRESSURE AND 500°K.  
 Graphite was omitted from the equilibrium in the first column. Graphite and all aromatic compounds were omitted from the equilibrium in the second column. Under these conditions, aliphatics are formed in high concentration.

	Aromatics Included	Aromatics Deleted	Aromatics Included	Aromatics Deleted
H <sub>2</sub>	.94x10 <sup>-4</sup>	.96x10 <sup>-6</sup>	Allene	.35x10 <sup>-17</sup>
O <sub>2</sub>	<10 <sup>-38</sup>	<10 <sup>-38</sup>	Ketene	.86x10 <sup>-13</sup>
H <sub>2</sub> O	.11x10 <sup>-3</sup>	.95x10 <sup>-8</sup>	Formaldehyde	.20x10 <sup>-11</sup>
CO	.41x10 <sup>-2</sup>	.29	Acetaldehyde	.75x10 <sup>-11</sup>
CO <sub>2</sub>	.61	.38	Formic Acid	.13x10 <sup>-10</sup>
Methane	.38	.32	Acetic Acid	.20x10 <sup>-8</sup>
Ethane	.66x10 <sup>-4</sup>	.46x10 <sup>-2</sup>	Butyric Acid	.30x10 <sup>-14</sup>
Propane	.80x10 <sup>-7</sup>	.46x10 <sup>-3</sup>	Octanoic Acid	.14x10 <sup>-25</sup>
Butane	.21x10 <sup>-9</sup>	.99x10 <sup>-4</sup>	Nonanoic Acid	.83x10 <sup>-29</sup>
Pentane	.29x10 <sup>-12</sup>	.11x10 <sup>-4</sup>	Palmitic Acid	<10 <sup>-38</sup>
Hexane	.47x10 <sup>-15</sup>	.15x10 <sup>-5</sup>	Methanol	.21x10 <sup>-12</sup>
Heptane	.73x10 <sup>-18</sup>	.19x10 <sup>-6</sup>	Ethanol	.86x10 <sup>-14</sup>
Octadecane	<10 <sup>-38</sup>	.15x10 <sup>-16</sup>	Octanol	.15x10 <sup>-31</sup>
Cyclopropane	.76x10 <sup>-13</sup>	.42x10 <sup>-7</sup>	Acetone	.51x10 <sup>-11</sup>
Cyclobutane	.23x10 <sup>-11</sup>	.11x10 <sup>-3</sup>	Dimethyl Ether	.51x10 <sup>-18</sup>
Cyclopentane	.13x10 <sup>-11</sup>	.48x10 <sup>-2</sup>	Lactic Acid	.87x10 <sup>-22</sup>
Cyclohexane	.15x10 <sup>-13</sup>	.46x10 <sup>-2</sup>	oxalic Acid	.65x10 <sup>-13</sup>
Ethylene	.88x10 <sup>-8</sup>	.59x10 <sup>-4</sup>	Pyruvic Acid	.71x10 <sup>-28</sup>
Propene	.53x10 <sup>-9</sup>	.29x10 <sup>-3</sup>	Glycerol	.71x10 <sup>-38</sup>
Butene	.92x10 <sup>-12</sup>	.42x10 <sup>-4</sup>	Carbon Suboxide	.24x10 <sup>-27</sup>
Octene	.21x10 <sup>-23</sup>	.43x10 <sup>-8</sup>	Benzene	.96x10 <sup>-4</sup>
Acetylene	.55x10 <sup>-16</sup>	.36x10 <sup>-10</sup>	Naphthalene	.73x10 <sup>-4</sup>
Propyne	.29x10 <sup>-16</sup>	.16x10 <sup>-8</sup>	Asphalt	.11x10 <sup>-1</sup>
Octyne	.15x10 <sup>-30</sup>	.31x10 <sup>-13</sup>		

synthesis. Of the oxygenated compounds, acetone, acetic acid, ketene, and acetaldehyde are most stable. Acetone is about as concentrated as octane. Traces of long chain fatty acids are also predicted.

When benzene and the other aromatics are included in this equilibrium, they are the most important organics. Higher homologs of all other families rapidly vanish. The ethane-to-methane ratio is  $1.3 \times 10^{-3}$ , and the concentrations of high homologs of the saturated hydrocarbons decrease by a factor of 300 for each increment in the number of carbon atoms. Here ethylene and acetylene are much less stable than ethane. These results are in qualitative agreement with the experimental results reported by Studier et al<sup>(9)</sup>, in which aliphatics rather than aromatics form when the temperature is kept sufficiently low. We take this as experimental support for the practical value of our method of limited equilibrium, in which under appropriate conditions, selected products are excluded from a system otherwise at equilibrium. Because of the greatly varying rates of different reactions, this method of computation may be suitable in many cases. Those reactions whose rates are commensurate with the time available will approach equilibrium sufficiently closely for an order-of-magnitude determination of the proportions of the products. Other, slower reactions will meanwhile have had only a negligible effect on the system. The validity of the computation, of course, depends on identifying the products which must be forbidden, as well as the major products which must be included.

### Plasma Experiments

Preliminary laboratory experiments which we have undertaken to test the above mentioned theoretical conclusions have yielded the predicted results. By means of a radio-frequency oscillator and the auxiliary equipment described in part previously<sup>(14)</sup>, it is possible to generate a plasma consisting of radicals, ions, and atoms from almost any compound having sufficient vapor pressure. When the energizing radio-frequency power is removed, such a plasma must tend toward a state of equilibrium, although the rapid rate of cooling may prevent its complete attainment. Compared to the time available during this cooling process, some reaction rates may be essentially zero, while others are relatively rapid. We believe that such conditions can be approximated by excluding from our computations certain compounds such as graphite, whose rate of formation is very slow. Since there are very abrupt changes in the concentrations of many compounds where the asphalt, hydrogen and oxygen thresholds of the general C-H-O ternary diagram (Fig. 1) are crossed, it should be possible to map out experimentally the main features over the entire range of this diagram. The effects of other elements on the final composition of the systems may be similarly investigated.

Initial results with a simple carbon-hydrogen system indicate the presence of the asphalt barrier. Excitation of gases in which the ratio of hydrogen-to-carbon is less than four-to-one leads to the formation of tars consisting primarily of polynuclear aromatic compounds. Among these, pyrene, coronene and chrysene (Fig. 5) have been identified so far; fluoranthene (Fig. 5) is also apparently present. Only minute traces of elemental carbon have been

found. With water cooling we get practically all nonaromatic material, although products are at least partially unsaturated. In other words the system appears to act as a limited equilibrium where aromatics are slow to form. This result is interesting in light of the computed results in Table II where aromatics have been excluded in a simulated limited equilibrium. If the hydrogen-to-carbon ratio is somewhat greater than four-to-one, the system appears in the hydrogen-rich region of the ternary diagram and only gaseous products are obtained. A detailed report of this work will appear at a later date. These experiments seem to demonstrate the plausibility of our use of the concept of "limited thermodynamic equilibrium".

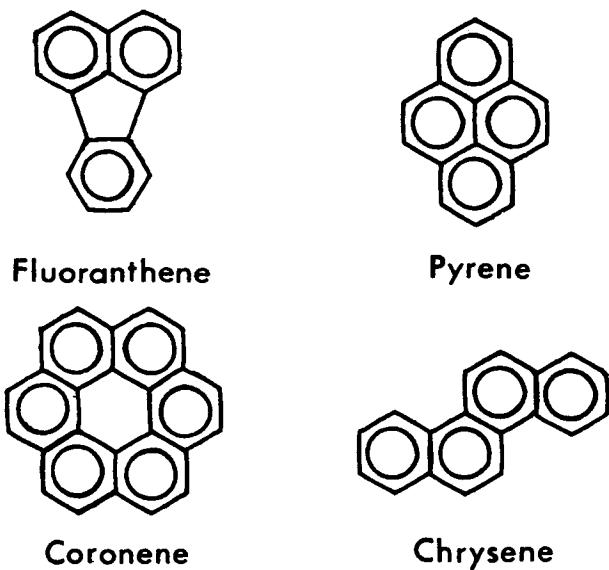


Figure 5. Compounds detected in products of plasma discharge reactions.

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## **Subject Index**

## SUBJECT INDEX

\* Indicates a figure, table, or sample calculation

Asphalt threshold, polynuclear aromatic formation	6,11*,184ff,185*,186*,226*,232* 233,234*,250,251*
Compound concentrations	14,16,18ff*,183*,185*,252*
Computational Method	2,3,171ff,189ff,221ff,229,244
Computer Program "CHEM-EQUILIBRIUM"	189
Earth, atmosphere	222ff,233*
Equilibrium constants	173ff
Errors	183,222
Experimental observations	
Plasma, discharges	6,184,238,255ff,256*
Standard free energies of formation	154ff*
Composition of meteorites	7,221,243ff,253
Fischer-Tropsch, heat catalysed reactions	6,184,243,253ff
Spectroscopy	219ff,223*,230*,236*,237*,239
Free energies	
Partial molal of the elements	14,17ff*,177ff,178*,180*,182*,186*
Standard, formation of atomic groups	14,15,166ff*,170,172ff,245
Standard, formation of compounds	14,15,154ff*,170ff,183*
Graphite phase boundary	4ff,5*,8*,9*,185,228*,232*,233,246*,247*,250
Ideal gas system, C, H, O	4,5*,17ff,245ff,246*,254*
Ideal gas system, C, H, O, N	41ff*,82ff*
Ideal gas system C, H, O, N, S, P, Cl	7*,64ff*,106ff*,250ff,252*
Jupiter, atmosphere	235ff,237*,239*
Limited thermodynamic equilibrium	3,13,248ff
Mars, atmosphere	233ff,234*,236*
Metastable systems	6,184ff,185*,186*,238,248
References	15,164,165,187,240,241,257
Standard states of elements	172
Ternary diagrams, explanation	4*,12ff*,16
Ternary diagrams, data	5*,7*,8*,9*,10ff,16,19ff*,226*,228* 232*,234*,246*,247*,249*,251*
Venus, atmosphere	225ff,226*,228*,230*,231,232*